DSRC
DEFENSE SCIENCES
RESEARCH COUNCIL

SUMMARY REPORT

of the

DEFENSE SCIENCES RESEARCH COUNCIL SUMMER CONFERENCE

La Jolla, California

July 1993

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Final Report compiled by
Charles Evans & Associates

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INTRODUCTION

This report is a summary of the 1993 ARPA-Defense Sciences Research Council Summer Conference which was held in La Jolla, California, during the period from July 6, 1993 through July 30, 1993. The report is being submitted to ARPA to enable them to utilize the results of the various workshops in a timely fashion. Later reports will be issued to include the materials generated at workshops held at periods other than those of the Summer Conference.

The principal task of the ONR-ARPA Grant is to bring together a group of the country's leading scientists and engineers for an extended period, usually the month of July to permit them to apply their combined talents to the planning and scoping of future materials research areas for the Department of Defense.

During the year workshops, and in some cases, program reviews, are attended by smaller groups of Council members and their reports are made directly to ARPA. This is a growing activity of the Council and these reports in the future will be included in the report submitted at the end of the contract year.

The technical direction of the Council is by a Steering Committee made up of seven representative members of the Council who work with ARPA management. The Committee for 1993 is given in the following table. The Steering Committee selects the relevant topics for the annual Summer Conference and works with the other council members in developing new areas in defense research. The membership on the Steering Committee and of the Council varies from year to year depending on the research areas that are of major interest to the Department of Defense. The Council membership for 1993 is given in the following table.

The Council also serves as a resource for other ARPA offices. The DARPA participants in the 1993 Summer Conference are given in the following listing.

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The agenda for the Summer Conference is prepared initially during the prior year's conference with input from ARPA and the Council. This is refined at subsequent Steering Committee meetings and the workshops are organized. The calendar year for the 1993 Summer Conference is shown in the attached figure.

July 1993

DSRC SUMMER CONFERENCE WORKSHOP SCHEDULE

MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
			1	2
5 *OPEN -- Travel*	6 *Sensing of Bio-Medical Data* Whitesides*	7 *Precision Assembly* Miller*	8 *Mixed Mode Electronic Packaging* Gilbert*	9 *Light Emitting Organics for Visible Display* Ehrenreich*, Wrighton
12 *Statistical Limits of Ultra-Small Devices* Ferry*, Osgood, McGill	13 *Statistical Limits of Ultra-Small Devices (am)* *Advanced Lithography (pm)* McGill*, Osgood, Ferry	14 *Advanced Lithography (continued)* McGill*, Osgood, Ferry	15 *ARPA DAY* Beasley*	16 *Real Time Process Control for Microelectronics Mfg* Hu*, Larrabee
19 *Environmentally Responsible Manufacturing* Larrabee*, Rapp	20 *Life Extension of Aging Structural Systems* Hutchinson*	21 *Prospects for Computations in Materials* Ehrenreich*, Patera	22 *Thermoplastic Matrix Composites* Economy*, Hutchinson	23 *Functional Organic And Organometallic Materials* Whitesides*
26 *Writing Day*	27 *Writing Day*	28 *Writing Day*	29 *Tutorial on Economics* Whitesides*	30 *Wrap-Up*

*Indicates Lead Coordinator

6/24/1993

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SENSING OF BIOMEDICAL DATA

George Whitesides

EXECUTIVE SUMMARY

Workshop Objective

This Workshop was convened to review aspects of technology relevant to the applications of information processing to selected areas in military medicine:

DoD Relevance

• **The delivery of sophisticated medical treatment in a military environment.** The *rapid* provision of the most appropriate therapy to injured personnel is a critical component in determining the outcome of treatment. Nine out of ten deaths in combat occur before medical care is provided; 50% of later deaths result from loss of blood. Giving the proper care for complex injuries as quickly as possible—certainly within an hour—is a major challenge in a combat environment. The development of technology for delivering appropriate care—even if it requires medical technology ordinarily reserved for central hospitals—is one focus of current planning in ARPA. The working hypothesis is that by applying information technology to medical problems, sophisticated care can be provided more rapidly and at lower cost. This approach puts a premium on devices for remote signal acquisition and analysis.

• **Monitoring the performance and capability of healthy personnel,** especially in combat situations, represents another challenge. Evaluating the ability of individuals to perform the tasks expected of them— whether in active combat or in decision-making capacities—requires both non-invasive technology for monitoring, and, perhaps more importantly, the knowledge base necessary to understand what to monitor and how to interpret the information produced.

• **Evaluation of the potential of military personnel to perform assigned tasks** is also a concern. Understanding the capabilities and limits of individuals would help both to define the most effective roles for them in military capacities, and also suggest environments in which they can be expected to perform best and most reliably.

• **Cost reduction** is an issue with all health care systems. Examining information technology for its ability to reduce costs in the military medical system has led to an active interest in the potential of the electronic medical record (EMR) both to increase the quality and timeliness of care, and to lower its cost. Further gain in effectiveness would be realize if the EMR is coupled to dual-use in the public medical sector.

Technical Summary

Phil Green (Telesurgery Corp.) outlined technology intended to enable surgeons to operate remotely. This technology has several components, all intended to be evolutionary (although potentially revolutionary in its overall impact on surgical practice) in order to minimize the time required to develop and introduce it. The two central components are the development of projection display systems based on stereoscopic laparoscopy, and of improved robotic manipulators to give the surgeon improved remote manual control of the operation of surgical tools. Communications systems intended to link the remote operating bench for the surgeon with the patient are also a significant component of the system. For civilian procedures, this bench would be co-located with the patient, so that the surgeon could intervene manually if required. In possible military missions, the separation between patient and surgeon might be substantial. This technology is part of the package being developed for the "operating theater in a Winnibago".

The technology that is now being developed focuses on supplementing the capabilities of surgeons in conventional laparoscopic procedures, and on the extensions of these capabilities. The current vision system provides a stereoscopic projection that appears to be acceptable in quality and definition; the robotic tools provide improved precision in manipulating laparoscopic devices. The surgeon at the remote operating bench is outfitted with transducers to provide a "hands on" feeling. The technology is at the point where it is being

demonstrated in "single-handed" mode, and will soon be extended to "two-handed" operation. A preliminary trial with a MASH unit proceeded well.

This methodology has the potential to serve as an excellent "test bed' to identify the needs for information processing and communications, and to define the parameters critical to the design of relevant communications and information processing systems. These parameters—required bandwidth, acceptable persistence and delay times for images and control loops—will impose constraints on implementation of remote procedures, and especially procedures that are "open" (that is, that involve large surgical openings, rather than the small openings characteristic of laparoscopy).

It is important to note several important constraints on the ultimate potential of remote surgery. First, in conventional laparoscopic surgery, the surgeon is present to deal with emergencies that may require opening the patient—e.g., unexpected bleeding. In the combat environment, where delay might mean death or irreversible damage, this constraint might not apply. Nonetheless, only certain types of procedures will be amenable to this type of procedure. Second, there are fundamental limitations in terms of physics that will provide constraints on the system. For example, the delay that would be involved in moving data over long distances may be unacceptable to the surgeons; thus, geographical proximity may be required to give some margin for fast reaction in difficult procedures. This type of limitation is, again, less serious for military applications, where any improvement in the level of medical care would benefit the patient, than it is in elective surgery for the civilian sector.

Steven Kornguth (Center for Human Performance, U. Wisconsin) reviewed the activities of this Center in correlating human performance with quantitative biochemical measures—neurological activity, metabolism, neuroendocrine activity, vascular activity—using techniques that ranged from MRI and PET to classical, non-invasive and unobtrusive techniques such as observation of gait, eye tracking and blinking, pupil response, and galvanic response. This work is important to the science base of the ARPA effort to monitor status in military personnel defining the parameters that correlate with human performance. An objective in ARPA is to evaluate the possibility of unobtrusive

monitors of performance status. At the present time, there is no clear understanding of what parameters should be monitored, much less how to monitor them. Attention has been focused on the parameters that *can* be measured: pulse, temperature, etc. The activities at this center should help to define both the most appropriate parameters correlating with performance, and the variance of these parameters with individual, environment and circumstance.

Kit Green (General Motors) reviewed the activities of the automobile manufactures in developing systems for monitoring the performance of drivers. Particularly interesting are two questions: Is the driver drunk, and is the driver drowsy or asleep? A large fraction of automobile accidents can be correlated with either alcohol impairment or with loss of attention through drowsiness. The company has used an interesting test population in examining performance under severe stress: viz., race car drivers. These individuals volunteer to have certain physiological parameters—heart rate, body temperature—measured, and these parameters have correlated with their racing performance. This type of study has the potential to provide a useful body of information in evaluating performance under very stressful circumstances, and to develop norms. For example, the pulse-rate of drivers may stay at 220 per min. for extended periods of time while racing (without appearing to compromise performance), and their temperature may rise to 104 F (albeit with substantial degradation in performance). both of these numbers would normally be associated with pathological conditions.

Chris Chute (Mayo Clinic) discussed medical informatics. The medical system generates an enormous amount of information,which is not presently managed efficiently. For example, it is usually necessary to retake medical histories when a patient moves from doctor to doctor, and the data from expensive tests—MRI and X-ray images—cannot be transmitted electronically. This primitive state of information processing in medicine has substantial monetary cost, both financially and the needed information about the patient is not available to the physician.

Problems in medical record keeping and in manipulating medical information in the military are, of course, much greater than in the civilian sector, since personnel move repeatedly and globally, since well-equipped medical

centers are not always available, and since time and communications channels are at a premium. An approach to simplifying the system is the Electronic Medical Record (EMR): a data file that would encapsulate all relevant medical information about an individual, and would travel with him or her. A system that would provide this information is extremely attractive in concept, but the design of such a system must address a number of fundamental issues.

Of these, the most important is the **representation** of medical data. There is now no standard format for recording me[illegible]l information, or even for describing a medical condition. Clearly, an EMR [illegible] be based on some representation of medical data, and the design of this representation must even precede the definition of the system in terms of capacity and architecture.

The design of an appropriate representation is a problem that has substantial political and sociological as well as technical components. Doctors must accept and use a specific, common representation, and this acceptance and use must be widespread. It is not clear what organization should take the lead in developing an appropriate representation for the EMR. The AMA is the largest professional medical organization in medicine in the U.S., and would be a logical candidate, was it not so conservative, Ludite and lethargic. The National Library of Medicine has a small program in the area, but this organization may not have the clout to sell a representation to physicians as a group. Insurance companies, HMOs and hospital collectives all have large financial interests in the form of any representation for medical data. In Europe, a system of representation has been developed that is more advanced than that in the U.S.; Europe has faced the problems of transmitting medical information across national and language borders for a long time. Perhaps an effort in the U.S. should start with the current protocols developed in Europe. Regardless of the mechanism, the development of a satisfactory representation or representations probably must underlie any substantial effort to develop advanced information/communication techniques in medicine.

Mel Simon (California Institute of Technology) summarized the current state of molecular genetics. There is no area of science in which advances have been more revolutionary in the last 20 years than genetics. The ability to identify known genes in humans is now relatively straightforward using techniques

such as the polymerase chain reaction (PCR), Southern blotting and the other methods of genetics. Most of the applications to date have been focused on identifying disease genes, and this activity is accelerating as the technology improves. In the foreseeable future, genetic techniques will be used to screen normal human populations for a range of susceptibilities and capabilities: for disease, to susceptability to stress, for specific patterns of behavior. At the moment, these issues are just beginning to be explored at the level of basic science, and the development of appropriate technology continues (in part under the banner of the human genome project). The development of methods for correlating genetics with characteristics of particular interest to the military is just becoming a practical goal. Whether ARPA should begin active work in genetics depends on an analysis of the opportunities and problems to which genetic information could be applied; the technology for many types of applications does, however, now exist.

The field of human genetics will introduce into biology an entirely new level of requirements for handling information. The human genome is approximately 3×10^9 base pairs in length. Although the relevant information from analysis of individual genomes will undoubtedly be stored in some form more condensed than an elementary, unedited sequence (probably as a listing of genes and associated characteristics), analyzing the quantity of information that will be generated in large studies of human genetics (particularly when the information now generated has a high—in the order of 1 %—error rate) will require new techniques.

Summary

A number of items emerged from the Workshop that represent issues or opportunities for ARPA in its initial efforts in biomedicine.

- Any effort to build an EMR will require the development of a specific representation of medical data. The proper strategy to develop this representation is a crucial component for planning a program directed toward an EMR.

- Concepts such as telesurgery require a more thoughtful and quantitative analysis of the communications requirements to provide a realistic basis for the design, costing and evaluation of an appropriate information processing system.

- The development of monitors for human performance status requires an understanding of what parameters to monitor, and how to interpret them. The science base in this area is still almost non-existent, and it is not even clear what types of data will be most useful: biochemically based information, characterizations from expensive instrumental techniques such as MRI, genetics, conventional psychological evaluation (or extensions of these techniques to more realistic, virtual-reality based environments) or some combination. It is important to understand what is being measured before moving too rapidly to design a measuring system.

- MRI is proving an invaluable imaging system throughout medicine. Handling the information processing required to generate, manipulate and transmit MRI images, and perhaps contributing to the hardware, represents an opportunity for some federal agency (although perhaps not ARPA). Improved MRI technology would have impact on many parts of the medical system, and would have substantial dual use value.

- The ARPA program in rapid field intervention in combat trauma will generate technology that is valuable in the civilian world as well, and especially in the handling of victims of automobile accidents. The dual-use aspect of this technology should be built into the ARPA program from the outset.

- The routine testing of personnel for genetic constitution will become possible in the next few years. ARPA should plan for the use of the flood of potential information from human genetics.

SENSING OF BIOMEDICAL DATA

George M. Whitesides

OBJECTIVE

- **To examine requirements and opportunities in information processing for military medicine**

RELEVANCE TO DoD

To help evaluate:

- ***information requirements for telesurgery*** and remote medical intervention
- the capability of ***sensors*** for trauma care, and for non-invasive evaluation of healthy personnel
- the potential of information for ***cost reduction*** in military health care
- the potential for ***spin-off of technology*** from military medicine into civilian health-care
- the ***science base for information technology in medicine.***

- **REPRESENTATIONS OF MEDICAL DATA ARE URGENTLY NEEDED.**

Most applications of information processing in medicine depend on the existence of a broadly accepted representation for the relevant data. No adequate representation now exists.

This problem is more organizational than technical. The interested parties are: insurance companies, HMOs, Medicare/Medicaid, the AMA, the National Medical Library. Representations are more highly developed in Europe than in the U.S.

- **INFORMATION REQUIREMENTS FOR REMOTE MEDICINE REQUIRE ENGINEERING DEFINITION.**

- **THE POTENTIAL FOR HUMAN GENETIC TESTING IN MILITARY MEDICINE IS ENORMOUS.**

Medical practice will be revolutionized by molecular medicine, especially molecular genetics. The DoD has not seriously addressed the potentials and problems of this technology in evaluating healthy individuals.

- **NON- OR MINIMALLY INVASIVE SENSORS OF PHYSICAL STATUS SHOULD BE DEVELOPED.**

At present, only primitive measurements (heart rate, blood pressure and pO_2, temperature) are available. It is not clear what parameters should be measured.

- **THE BASIS FOR PREDICTING "CAPABILITIES"— PSYCHOLOGICAL, IN MAKING DECISIONS, PHYSICAL — NEEDS SUBSTANTIAL DEVELOPMENT.**

- **CERTAIN MEDICAL/INSTRUMENTAL CAPABILITIES—ESPECIALLY MRI AND ULTRASOUND—MIGHT BENEFIT SUBSTANTIALLY BY APPLICATION OF MILITARY TECHNOLOGY.**

- **THERE IS AN OPPORTUNITY FOR APPLICATION OF INFORMATION TECHNOLOGY IN TRAINING OF ALL LEVELS OF MEDICAL PERSONNEL.**

- **AN ARPA PROGRAM IN MILITARY MEDICINE COULD HAVE BROAD IMPACT ON THE PRACTICE OF MEDICINE IN THE CIVILIAN SECTOR.**

(Automobile related accidents alone represent a cost of ca. $120 B per year in the U.S.)

NON-INVASIVE SENSING OF BIO-MEDICAL DATA

Workshop Coordinator: George M. Whitesides

July 6, 1993	
8:00 am	Introduction to the Workshop, George Whitesides (DSRC/ Harvard University), Ken Gabriel (ARPA), Frank Patten (ARPA), Ira Skurnick (ARPA)
8:30 am	"Telesurgery", Phil Green (Telesurgical Corporation)
9:30 am	"Human Performance — Neural, Whole Body, and Systems Strategy", Steve Kornguth (Center for Human Performance and Imaging Technology, University of Wisconsin)
10:30 am	Break
11:00 am	"Performance Sensing in Automotive Systems", Kit Green (General Motors)
12:00 Noon	Lunch
1:00 pm	"Medical Concept Representation", Chris Chute (Mayo Clinic)
2:00 pm	"Now That We Know the Sequence of Your Genome, What Do We Do With It?", Mel Simon (California Institute of Technology)
3:00 pm	Summary and Discussion
4:00 pm	Adjourn

SENSING OF BIO-MEDICAL DATA

July 6, 1993

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PRECISION ASSEMBLY

David A. B. Miller

Objective

This workshop focused on precision mechanical assembly and manufacture. It brought together a broad range of speakers, from industrial, academic, and research corporation backgrounds. The goal was to understand the issues in precision assembly in general, with a view to understanding the role ARPA could play in this field.

The focus was on the underlying problems common to precision assembly, regardless of the specific mechanical technologies or the size scale of the assembly. Hence the workshop did not discuss specific mechanical technologies in detail, nor did it discuss at any length the many emerging technologies appropriate specifically for micromechanical assemblies.

Relevance to DoD

Precision assembly is of direct importance in military applications. A specific current example is seeker heads for missiles. It will be of increasing importance for portable or hand-held equipment, such as personal gyroscopes and smaller global positioning system units, and in systems in which sensors are packaged with their mounting and their electronics. In the commercial market, examples of growing markets requiring precision assembly include portable mass manufactured items such as cameras, compact disk and tape players, and disk drives for portable computers. Precision assembly in general is clearly important for maintaining and improving national competitiveness in manufactured goods. Precision assembly is also clearly a dual use technology in which advances in commercial practice can result in lower cost and higher performance for military applications.

Scientific & Technical Issues

Issues in Precision Assembly

The issues identified in the workshop can be summarized in broad categories:

Design

An important component of the success of precision assembly is good design. Good physical technology will not compensate for poor design, and good design can result in very precise assemblies with comparatively simple technologies in many cases. Of course, such design must be design for assembly; the designer must understand the assembly process. Industrial experience shows also that the most successful precision assembled products have a continuing interaction between design and assembly as the product is optimized.

The methodology and the design tools for design of precision mechanical assemblies are weak when compared, for example, to those for design of electronic integrated circuits. This relative weakness partly reflects fundamental differences in mechanical assemblies compared to integrated circuits. Useful complex electronic circuits can be designed in a hierarchical fashion, as circuits that are made by combining other circuit blocks. Mechanical assemblies generally cannot be designed this way; the component parts typically have multiple functions, and the design of one often cannot be isolated from the design of another. In addition, mechanical assemblies are usually also three-dimensional rather than a set of planar layers, the parts may move in use, and the design must allow for wear.

There are tools available for computer-aided mechanical design, and there are usable methodologies for optimizing design to improve the precision of the final assembly, but this clearly an area that could be developed further. Since good design is crucial for successful precision assembly, such tools and methodologies could be very important for sustaining a competitive US position, just as the comparable tools in electronic design help the US maintain a strong position in certain semiconductor products. In general, including the electronics area, design tools that bridge the gap between the system concept level and the design of individual parts are weak.

An additional problem in the design of very small assemblies is that the science on small scales, although well-known in principle, may present different issues from that on larger scales. Designers are generally not so familiar with such small systems, which makes their design more difficult.

Education and Training

Training in the skills and attitudes required for precision assembly and manufacturing in general has several weaknesses.

- Success in mass manufacturing in general requires a value-driven rather than performance-driven approach, and this should be emphasized more in educating scientists and engineers.
- Education for any kind of manufacture, including the education of designers, should involve "hands-on" experience on an assembly line. Otherwise the designer will not understand the issues of design for assembly.
- Training of "craftsmen" is important. There is ultimately no substitute for expert knowledge and skill to extract the best from any technology. Industry has an important role in this education.
- In general, corporations have to be actively involved in the education for manufacture because they know most about it and have the most to gain from it, and many already are.

Precision Mechanical Technologies

Although this workshop deliberately did not concentrate on specific mechanical and assembly technologies, these are clearly important. Arguably one of the reasons why electronic integrated circuit design is relatively successful is that it does not need often to be very optimized; the designer can rely on rapid improvements in technology, rather than optimization of the design within a technology, to improve the performance of the system. Clearly, improvements in mechanical and assembly technologies could improve precision assembly, although discussion of these was beyond the scope of this particular workshop.

Value System

There are several problems related to value systems in academic research, in education, and possibly more generally in US society, which work against successful precision assembly in the US.

Although product design is crucial to precision assembly, the final assembly can only be done competitively if the assembly processes are themselves optimized.

- If this optimization is to work, it requires that process engineering is respected and that engineers regard this as just as important as design. There is a perception that design has all of the "glory".

- The process of optimization has to be continued over a long period. It requires a persistent and unremitting attention to detail. Citizen Watch Company of Japan has made a successful business out of precision assembly by refining and exploiting screw assembly machines over decades. It still uses some machines that are decades old. It will be the mass manufacturer for some precision mass-market assemblies designed in the US.
- Focus on individual glory is perhaps counterproductive for the optimization of manufacturing processes.

The peer review system in academic research is arguably not very successful at encouraging work that is relevant to precision manufacture. Such work can be intellectually challenging and can involve breaking new ground, but it does not fit readily within the recognized academic disciplines, especially the scientific ones. The understanding among academic scientists of the real underlying long-term problems related to manufacture is not at a high level, and is not ameliorated by the lack of communication between the academic and manufacturing communities. Without such understanding, however, the peer review process cannot be as successful. Furthermore, manufacturing is not an area that is strongly driven by publications, and hence the academic valuing of publication record is not likely to help this area.

Infrastructure

Specialized Small Companies

Small companies are very important in the precision assembly business. They often have the key specialized technologies needed. They are, however, very vulnerable to being destroyed if they are taken over by larger companies, and it is very difficult to resurrect them if this happens. They are also very vulnerable to short-term economic swings that cause delay or cancellation of orders. Although the direct economic impact of the loss of one such small company may not be large, the indirect impact can be considerable, forcing customers to go overseas in many cases, and damaging the local infrastructure that nurtures manufacturing in general.

Communications and Information Infrastructure in the Community.

- The communications between the manufacturing and academic

communities is weak. Academics in general are not well connected to the problems of manufacture. If they are not well informed in this area, they will not know what the underlying problems are, they will not choose research directions that are most likely to bear on those problems, and they will not be educating their students in these areas. This communication needs to extend beyond the traditional manufacturing science and engineering areas into the scientific disciplines. Traditional academic journal publishing does not appear to be a useful mechanism for communication between the academic and manufacturing communities.

- There is a need for a database of information and catalogs of precision components and suppliers. Much of the success of an assembly can depend on having the best information in choosing components. Handling the hardware for this task is probably not the largest problem; a key underlying issue is that there is not a standardized description language (a "representation") for mechanical components.
- There is a lack of a forum through which those involved in the precision assembly business and those who wish to learn more about it (such as academics) can informally exchange information. A simple bulletin board or e-mail group on which people can openly post general queries and information could be a partial solution. Such e-mail groups are operating successfully in other fields.

Possible Areas for ARPA Involvement

The areas where ARPA could be effective include

- research on specific topics
- communications infrastructure
- the value system

By its selection of which projects are funded, it can strongly influence the value system.

- education

ARPA, especially in conjunction with other agencies, could also be effective in educational programs.

Specific Recommendations for ARPA

Research Programs

ARPA should consider a program in design tools and methodologies. This program should address

- mathematics
- design methodologies
- system representation methods
- computer-aided analysis and design tools for the design of complex, three-dimensional mechanical systems

ARPA should also actively continue to address specific microassembly and micromechanical technologies.

Infrastructure

ARPA should explore the possibility of an e-mail forum, using Internet as a backbone, to improve informal communications among the manufacturing and academic communities.

ARPA should also consider how a database of information on precision mechanical parts and assemblies might be usefully operated.

PRECISION ASSEMBLY

D. A. B. Miller and A. Heuer

Objective

- Understand the issues in precision assembly in general
- Focus
  - Underlying problems regardless of the specific mechanical technologies or size

DoD Relevance

- Precision assembly is of direct military importance, e.g. seeker heads for missiles
- Increasing military importance for portable or hand-held military equipment, e.g. personal gyroscopes, smaller global positioning system units, integrated sensor/mounting/electronics systems
- Increasing commercial importance in mass-manufactured portable items, e.g., cameras, compact disk players, disk drives for portable computers
- Clearly important for maintaining and improving national competitiveness in manufactured goods, and as a dual-use technology.

Design

- Good design is crucial for precision assembly
- Design must be design *for assembly*
- Continued interaction between design and assembly is crucial
- Methodology and design tools for precision mechanical design are weak
  - Fundamentally different design problem compared to integrated circuit design
    - Mechanical design is not hierarchical
    - Design of one part influences design of another
    - Mechanical parts must perform many functions
    - Mechanical design is three-dimensional, and parts move and wear
- Better design tools and methodologies could have significant impact on US abilities in precision assembly and manufacture

Education and Training

- Value-driven rather than performance-driven design approach should be emphasized
- Education should involve "hands-on" assembly experience on an assembly line
- Training of "craftsmen" or experts is important to extract the best from any technology
- Corporations must be actively involved in education for manufacture

Precision Mechanical Technologies

(although important, they were not covered by this workshop)

Value System

- Process engineering is just as important as design engineering for making a mass-manufactured precision product, but it has no "glory"
- Sustained attention to detail is essential for precision assembly
- Academic peer review system is not well suited to encouraging work relevant to precision manufacture

Infrastructure

- Specialized small companies very important, but vulnerable to destruction, especially when taken over
  - Weakens manufacturing infrastructure
- Communications and information infrastructure
  - Communications between the manufacturing and academic communities is weak.
  - There is a need for a database of information and catalogs of precision components and suppliers
    - Problem — there is not a standardized description language (a "representation") for mechanical components.
  - Lack of a forum for informal communication within the precision assembly community and out to the academic community (e.g., an e-mail bulletin board or group)
- Needs
  - Intellectual underpinning (a "paradigm") to provide systematic methodology for incorporating precision assembly into the design process

Areas for Possible ARPA Involvement

- Research on specific topics
  - CAD tools?
  - Design systems?
  - Neural net controllers?

- Communications infrastructure

- The value system
  - By its selection of which projects are funded, it can strongly influence the value system.
  - Specifically, highlight issue of precision assembly at contractors' meetings
  - However, issue of manufacturing and the environment cannot be ignored

- Education
  - ARPA, especially in conjunction with other agencies, could possibly be effective in stimulating educational programs, e.g. workshops, short courses

Specific Recommendations for ARPA

Research Programs

- ARPA might consider a program in design tools and methodologies. This program could address
  - Mathematics
  - Design methodologies
  - System representation methods
  - Computer-aided analysis and design tools
    - For the design of complex, three-dimensional mechanical systems
    - ARPA should also actively continue to address specific microassembly and micromechanical technologies.
    - Specifically consider element of precision assembly in more ARPA programs

Infrastructure

- Explore the possibility of an e-mail forum
- Consider how a database of information on precision mechanical parts and assemblies might be usefully operated.

PRECISION ASSEMBLY

Workshop Coordinator: David A. B. Miller

July 7, 1993

8:00 am	Introduction to the Workshop, David Miller (DSRC/AT&T)
8:15 am	"Precision Micro-Assembly," Peter Will (USC ISI)
9:00 am	"Some Fundamental Issues in Complex Precision Mechanical Product Design and Assembly," Dan Whitney (Draper Labs)
9:45 am	Discussion
10:00 am	Break
10:15 am	"Design Issues in High Speed Precision Machines," Alex Slocum (MIT)
11:00 am	"Small, High-Technology Business Viewpoint on Precision Assembly," Ted Arneson (Professional Instruments)
11:45 am	Discussion
12:00 Noon	Lunch
1:00 pm	"Precision Mechanical Assembly Issues in Polaroid Photographic Products," Bill Plummer (Polaroid)
1:45 pm	"Contrasts between Japanese and American Approaches to Precision Mass Assembly," Ray Tussing (Hewlett-Packard)
2:30 pm	Discussion
4:00 pm	End of Workshop

WORKSHOP SPEAKERS

The speakers at the workshop were:

Peter Will (USC Information Sciences Institute) Peter Will has a broad industrial experience in several major corporations. He discussed mechanical assembly in general, and briefly reviewed some current micromechanical research work;

Dan Whitney (Draper Labs) Dan Whitney discussed the issues of design for precision assembly, emphasizing the differences between the hierarchical design possible in electronic systems (especially integrated circuits) and the multifunctional design necessary in precision mechanics;

Alex Slocum (MIT) Alex Slocum discussed some of the formal design approaches that can be applied to improving the overall precision in complex and high-performance mechanical assemblies;

Ted Arneson (Professional Instruments) Ted Arneson brought a long and broad experience in precision assembly from the perspective of a small corporation specializing in this field. He emphasized the importance of education, training, and craftsmanship, and the necessity of long-term corporate commitment, for success in high precision work;

Bill Plummer (Polaroid) Bill Plummer discussed the various principles required in practice for a successful precision mechanical assembly that can be mass manufactured, and illustrated these by example from three generations of Polaroid folding cameras;

Ray Tussing (Hewlett-Packard) Ray Tussing discussed the process of bringing a leading-edge, high-volume, precision mechanical product to mass manufacture in a short time scale, illustrated through his experience with a 1.3 inch hard disk drive product. He discussed the necessity of bringing together the experience and technology of large and small corporations to accomplish this, and detailed particularly the contrast between Japanese and American corporations in precision manufacture.

PRECISION ASSEMBLY

JULY 7, 1993

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MIXED MODE ELECTRONIC PACKAGING

Barry K. Gilbert, L. Eric Cross

EXECUTIVE SUMMARY

INTRODUCTION

On July 8, 1993, the DSRC held a one day workshop on the need for mixed mode electronics, and mixed mode electronic packaging, as the decade progresses. We will first define mixed mode electronics, then describe the thrust of the workshop presentations, and thereafter make recommendations for possible approaches that ARPA can use to assure that the appropriate technologies are pursued.

Silicon bipolar chips, and more recently GaAs MESFET chips, are being used increasingly in high performance system designs; the 200-350K gate GaAs digital chips are even beginning to challenge silicon ECL as the technology of choice for high performance digital systems, while GaAs is already the clear technology winner over silicon in an increasing number of analog microwave applications. These recent trends are now virtually irreversible. An additional emerging trend is the combining of digital subsystems in the same chasses or circuit boards with analog subsystems, in a variety of applications. Many of these combined digital/analog, or mixed mode electronic systems, tend to operate at high signal center frequencies and/or signal bandwidths and, simultaneously at high system clock rates. The high frequency nature of such systems will create challenges for the designers of the electronic components themselves, but also for the designers of the electronic packaging for the components.

The purpose of the workshop was to assess the likely growth of mixed mode electronics, to evaluate whether electronic packaging for mixed mode electronics was progressing satisfactorily, or whether there are significant technological "holes" in the component or packaging technologies. To review the electronic systems field, we invited speakers from the Air Force radar community (Mr. Frank Lamb, Wright Laboratories); from the National Security

Agency group working on long haul fiber optics and satellite data transmission (Dr. William Semancik); from an aerospace corporation (Raytheon Electromagnetic Systems Division) working on a variety of radar and electronic warfare (EW) applications (Dr. Beshad Basegi); and from the civilian telecommunications industry (Mr. Reg Simpson of Northern Telecom). To help us evaluate the state of the art of the electronic packaging technology particularly with regard to its ability to support mixed mode electronic systems, we invited two individuals responsible for existing electronic packaging fabrication facilities (Mr. Phil Trask, Hughes Aircraft Corporation and Mr. Mike Gdula, General Electric Corporate Research and Development Center). To assist us in an evaluation of materials technology issues, we heard from: 1) Dr. Eric Cross (of Penn State Materials Research Laboratories and a member of the DSRC), who discussed the state of development of so-called high-K dielectrics (materials with dielectric constants in the range of 100-30,000); and 2) Dr. Paul Kohl of Georgia Tech, who discussed the state of development of metallurgy and low-k dielectrics for electronic packaging targeted for mixed mode applications. A more detailed description of the presentations appears in the Appendix; we will summarize the outcome of this meeting in the following paragraphs. References from the literature and lists of published papers for further reading are available on request from the authors of this report.

I. Potential Applications of Mixed Mode Electronics and Mixed Mode Packaging

An increasing number of designers from the digital and analog processor world are requesting even more speed, and they are looking increasingly at the possibility that GaAs (and even InP) HBT's will come to their assistance. These groups include the designers of fiber optics transceivers, the Air Force (with their ten year Digital X-Band Radar project), the designers of optical up-, down-, and cross-links for satellite communications, the error detection and correction (EDAC) community, the strategic and tactical jammer community, the nascent wideband COMSAT community (as represented by the ARPA/NASA Advanced Communications Technology Satellite Program), the electronic warfare (EW) community, and the INFOSEC community, to name the more apparent members of this group (Figures 1 and 2). At least one interesting example of critical technology mixed mode electronics in which speed/bandwidth is NOT an issue is full

authority digital engine control (FADEC) for aircraft engines.

It became evident through the course of the workshop that there is no question that mixed mode electronics is rapidly becoming a requirement for future systems. Rather, the unknown factors are the rapidity with which mixed mode electronics will make its debut, and which supporting technologies are insufficiently developed to allow a rapid infusion of mixed mode designs into next generation electronic systems.

II. Most Likely Packaging Approaches for Mixed Mode Electronic Systems

Conventional approaches to the packaging of integrated circuits, in which individual integrated circuits are separately packaged in dual inline packages (DIPs), flat packs, or leadless chip carriers, and then attached to conventional printed circuit boards, simply will not work for high performance digital components; nor will this approach work for wide bandwidth analog systems. The analog community has for many years attached multiple unpackaged chips to ceramic substrates, and wire bonded the chip pinouts to traces on the ceramic substrates in an approach referred to as hybrid packaging. Hybrid packaging was adapted in the 1960s for analog systems because the frequency performance degradation and packing density losses associated with single chip packaging could not be tolerated. While more costly to assemble, the hybrid packaging does not give up performance due to parasitic reactances of the single chip packages, nor propagation delay problems associated with the long metal traces buried in the single chip packages.

Since the mid 1980s an evolution of hybrid packaging has been under development for digital chips as well, using a technique to fabricate the substrates which relies on organic dielectric and metal layers laid down on a mechanical support. The organic layers have typically been spin or spray coated and then cured, and the metal layers have been sputter deposited and then plated, followed by lithographic patterning. Up to eight metal layers have been demonstrated using this approach, whose heritage is clearly from the integrated circuit industry, rather than the classical printed circuit board industry. These so-called multichip modules (MCMs) have demonstrated line geometries much finer than feasible for printed

circuit boards, e.g., 8-25 micron wide lines versus 5-8 mil wide lines. In actual studies, area reductions of 25:1 and weight reductions of nearly 10:1 have been demonstrated for systems implemented in single chip packaging and printed circuit boards in comparison to an MCM implementation (the system in question was an all-Gallium Arsenide implementation; see Figure 3). Even greater packaging density improvements than the 25:1 number are definitely achievable. In addition, the conformations of the signal waveforms measured from these MCMs are almost textbook in their quality (Figure 4).

Multichip modules are thus viewed as the natural packaging candidate for mixed mode systems rather than single chip carrier and printed circuit board packaging. Performance gains similar to those already demonstrated for digital systems, and for a small number of purely microwave systems, are definitely feasible for mixed mode systems through the use of MCM packaging technology. However, the present state of the art of the MCM technology is being developed primarily for digital components operating in the 100 MHz clock rate environment, typically based on silicon CMOS technology. As a result of this orientation, little or no attention has been given by MCM fabricators to the special requirements of high performance digital and mixed mode systems designers. This mindset will have to change if the evolution of mixed mode electronic systems is not to be hampered by inadequate packaging technology.

III. Areas Requiring Development To Support Full Capability Mixed Mode Electronics

Several subtechnnolgies require further development to support mixed mode electronics. They are: 1) Computer aided design, layout, and simulation tools for mixed mode systems; 2) Development of improved dielectrics compatible with MCM fabrication processes, in particular, very low permittivity materials (to improve shielding and allow flexibility in the design of interconnect line impedances over the range of, e.g., 30-75 ohms) and very high permittivity materials (to support embedment of large value decoupling capacitors directly into the MCM substrates); 3) Development of improved, lower sheet resistance metals systems and recipes for thicker metal lines (3-5 microns is common, but 5-10 micron thick lines are

needed) compatible with MCM foundry processes, with the intent of: a) substantially lowering the signal loss in interconnects, b) lowering the distribution losses in the power and ground planes buried in the MCMs, and c) increasing the number of metal layers which can be incorporated into the MCMs (five metal layers is common, eight layers have been demonstrated, and 10-12 layers are needed for additional power and shield planes in mixed mode MCM structures; see Figure 5); 4) The ability to integrate special structures, such as highly accurate resistors, integral inductors, and capacitors (in addition to those capacitors employed for power-ground plane decoupling, i.e., local charge storage), directly into the MCMs. Several of the more salient points will be expanded upon below, with the areas considered the most urgent presented first.

a. Improved Computer Aided Design and Simulation Tool Suites

It was unanimously stated by the workshop participants, particularly those from the systems community, that there is a paucity of design, layout, and simulation tools for the mixed mode electronic environment, and specifically for mixed mode electronic packaging problems.

The vast majority of DIGITAL design, circuit simulation, logic verification, and chip layout tools are targeted for the 100 MHz silicon CMOS community, and concern themselves not at all or very little with the needs of high speed chip designers. The tools available to the ANALOG MICROWAVE community do not deal with wideband digital problems, but instead concentrate primarily on high frequency, narrowband or low modulation index problems. Individual design, layout, and simulation tools for the wideband digital environment are in short supply, and integrated tool suites are nearly nonexistent.

Finally, tools which are capable of combining low level and/or high frequency analog chips and fast digital chips on the same module, while accounting for issues of signal matching, impedance control, power and ground plane integrity, etc., etc., to create a true mixed mode environment, are definitely not to be found. The development of individual tools for mixed mode environments, as well as integrated tool suites for these environments, is definitely of the highest priority.

b. Improved High and Low Permittivity Dielectrics Compatible with MCM Foundry Recipes

<u>High Permittivity Dielectrics</u>

For high density high speed MCMs there is urgent need to replace the discrete capacitors which provide local charge (current) to guard against "power rail collapse" and/or "ground bounce" with fluctuating current demand from the integrated circuits on an MCM during each switching cycle. The present discrete capacitors use up valuable space, are expensive to install, and their interconnect and internal electrode architecture add resistance and inductance which severely limit upper frequency response.

The demonstration that large area sheet capacitors can in fact be effectively incorporated into MCMs was recently provided by nCHIP through a contract under the auspices of the present ARPA/ESTO Physical Packaging Initiative; power and ground plane noise levels on a set of 16-chip GaAs modules has demonstrated one of the lowest levels of power and ground plane noise (approximately 25 mV p-p; see Figure 4) ever observed in these structures. However, though the thickness of the dielectric was 2000 Angstroms, the dielectric (aluminum oxide) had a relative permittivity of 11 and provided approximately 50 nF/cm^2, which is not nearly high enough: The chip packing density of these modules was very low, and could have easily been increased by a factor of four or more, in which case the noise levels would have become unacceptibly high at 100 mV p-p or greater. Clearly, much higher levels of local charge storage will be needed as mixed mode modules become denser and faster.

Ferroelectric and ferroelectric-like dielectrics offer the maximum stored energy density and in thin film form can provide the possibility for adequate single sheet capacitance (~0.1 to 1 fF/micrometer2) to provide low inductance local charge (current) density under the power plane of the MCM. Dielectric nonlinearity, which is endemic to all ferroelectric-based systems, suggests that the local charge delivery for a given tolerable voltage drop may be improved by moving from the simple ferroelectric, to a relaxor ferroelectric and ultimately to a phase switching dielectric based on a suitably chosen antiferroelectric (Figure

6). Well characterized film compositions are available in the lead zerconate titanate, lead magnesium niobate, and lead stannate zirconate titanate composition systems to address each of these needs.

It will be important to determine upper frequency limits to discharge in each of these systems; however, the displacive (soft mode) behavior for these ferroic systems suggest that upper frequency limits may be above 10 GHz (.1 psec).

For so-called "chips last" MCM technologies (in which the MCM substrates are fabricated and the chips are then installed, much like a miniaturized circuit board), the stable inorganic package (aluminum nitride, glass ceramic, silicon, etc.) will provide an effective substrate for ferroelectric film deposition and annealing, which must be carried out in the range of 450-650 C. In GaAs "chips first" packages (in which the chips are placed in wells milled out of the ceramic support substrate and the power planes and interconnect layers are deposited on top of the chips), it may be necessary to lay the capacitor film onto the substrate before the chips are placed.

In flexible polymer based interconnect systems there are needs for local high capacitance. Since there are no high permittivity polymers it may be important to explore polymer ceramic composites where the permittivity level may be enhanced by an inorganic ferroelectric component. In such composites the effective permittivity of the mixture depends critically on the self connections (connectivity) of the phases. This connectivity can be controlled by electrophoretic/dielectrophoretic methods in the liquid phase of the monomer and trapped in place by the polymerization reaction.

Dielectrophoretically induced chaining offers the possibility of designing in locally varying permittivity or permeability to enhance the functionability of the polymeric component.

Low Permittivity Dielectrics

The increasing clock rates in high speed MCMs and the need to maintain characteristic impedance carry a continuing need for the further development of lower permittivity dielectrics for interconnect structures in both "chips first" and "chips last" technologies. At present,

polyimides are widely used because of their availability and thermal stability; however, the permittivity of approximately 3.4 is too high and the thermal expansion/thermal stress characteristics strongly limit the number of layers which can be laminated.

c. **Improved Metallurgy Recipes (Including Metal Systems for Integral Resistor Structures)**

High Conductivity Metals

Copper and aluminum are widely used for the interconnect structures in MCMs and other packages. However, with processes such as vapor deposition or electroplating, thin films develop higher resistivities than the bulk metal. Losses measured in copper and aluminum lines on MCMs are higher than desired (Figure 7, upper panels); remedies which can decrease these losses are sorely required. In silver, electroplated layers retain the full conductivity of the bulk metal; also, elastic stresses are less in silver than in copper, aluminum, or gold.

Two problems exist for the more widespread use of silver: firstly, the propensity for electrochemical migration in any moisture film, and secondly corrosion associated with the formation of sulphides. Both problems can be addressed by full hermetic sealing of the structures. For silver, the cost disadvantage over base metals is vanishingly small.

Thicker Metal Layers

Techniques must also be developed for creating lines much thicker than the 3-5 microns presently used, as thicker lines will decrease resistive losses of both the DC variety (straight ohmic losses) and the AC variety (i.e., AC, or skin effect, losses can be decreased by thicker thicker lines in MCMs because of a peculiarity of the skin effect condition in lines whose thickness is on the order of the skin depth, as is the case for MCM interconnects; see upper panels of Figure 7). The thicker lines in turn cause planarity and stress buildup problems in the dielectric layers, which must be solved through better dielectric materials with lower stress levels and better planarization characteristics (thus demonstrating that the various elements of these problems are not decoupled).

Low Conductivity Material Formulations

Because integral resistors are required for transmission line terminators and other electrical circuit components on mixed mode MCMs, the ability to lay down resistors with high accuracies (minimum 5%, best case 1% or better), work needs to be done to assure that thin film tantalum nitride, tungsten silicide, or other formulations of resistors can in fact be laid down with the required accuracies. Amazingly, such processes, though known for many years, are NOT under control; the best as-deposited integral resistors are at present not better than ±20%. Although such resistors can be laser trimmed, the trimming process is a difficult additional fabrication step which increases costs and decreases MCM substrate yield.

High Permeability Metals

The ability to deposit materials with high permeability would improve the ability to incorporate inductive components, such as inductors and transformers, directly into the MCM substrates.

d. **Development of a set of mixed mode demonstration modules or subsystems suitable for insertion into real world, already fielded, electronic systems.**

Finally, as was learned in the 1980s in the DARPA/DSO GaAs Pilot Lines and the GaAs Insertion Program, new technologies tend to infiltrate slowly into the electronic systems community without a demonstration that the technology, whatever it is, has become sufficiently mature to be incorporated into systems with low risk. Thus, an insertion program for mixed mode electronics in general, and mixed mode Moms specifically, could make the transition toward mixed mode electronics proceed much more rapidly than without the demonstrations. The demonstration modules to be fabricated in this portion of the effort could easily be drawn from the test instrumentation, radar, WE, lanolin telecommunications, or combust industries; many examples of such systems were provided throughout the workshop.

The recommendations presented above are summarized in Figures 8 through 11.

APPENDIX

Applications for Mixed Mode Electronics

Radar

The Air Force representative pointed out that the radar community is working on two areas of development. First, the new CM technology is being exploited to produce Transmit/Receive (TR.) modules which will have enhanced performance and significantly decreased costs, down from the current $2000/module to $400/module. The F-22 aircraft will employ 2000 TR. modules for conferral applications, each running at 4-10 watts power output. Batch fabrication is being attempted to keep costs down, and to increase uniformity; hand tuning of each module is unaffordable. Known good die are a key to low cost manufacturing. Thermal management is a significant problem. The frequency band of greatest interest is X-band, i.e., 8-12 GHz. They would like to have three dimensional modules with analog RF chips on one layer of the stack, digital chips on another, with RF interconnects between them; wafer level processing, and affordability, in very thin modules. No individual CAD tools are available to design mixed mode ICs, and even fewer integrated CAD tool suites for mixed mode applications. In the 3D structures, each layer would be fabricated and tested separately, and only then assembled into a stack.

The long term goal of the Air Force, by the year 2002, is digital X-band radar, in which incoming radar signals would be digitized directly at the receiving antenna at 20 gigasamples/sec, and processed entirely digitally thereafter; the same approach would be used on the transmission side of the radar. Digital beamforming on both transmission and reception represents a holy grail of sorts for the Air Force radar community.

The aerospace community working on radar and EW applications have a requirement for operation in the .5-18 GHz regime; data rates are very high. Analog channelizers have problems of stability, reliability, and cost; they want digital receivers with low cost and broad bandwidth; such digital receivers will then be usable in many applications. The Raytheon participant stated that such functionality at acceptable cost and with desired performance is not achievable without mixed mode MCMs. Both comint and elint receivers are also being developed in the 1.55-2.95 GHz frequency band using MCM technology. Direc-

tion Finding (DF) capability is also required; in a system presently under development, 27 conventional printed circuit boards would be required to implement the desired functions. The chips are presently silicon, but GaAs MESFETS and HBTs are rapidly being incorporated into new designs, and InP HBTs will be incorporated into systems in the future. A/D converters are very important in these applications; Raytheon plans to employ the 3 gigasample/sec A/D Converters under development by ARPA/MTO. Conversion to digital implementations will allow set-on receivers to do away completely with expensive analog delay lines, each of which costs $.25-2.5 million. The digital MCMs which perform some of these functions have 128 inputs and 128 outputs at 400 MHz each. Clock rates in some modules are GHz clock rates, with 100 psec edge speeds. The presenter from Raytheon pointed out that twenty eight separate companies have expressed interest to Raytheon in the use of mixed mode electronics and mixed mode MCMs, covering a very wide range of applications, and a wide range of frequencies.

Telecommunications

The government communications presenter indicated that a variety of Synchronous Optical Network (SONET) protocols are in place, with 2.5 gigabits/sec common now for fiber protocols; a 9 gigabit/sec protocol (OC-192) will be defined this year. However, a data rate hierarchy has been recognized: gigabits/sec to the theater of battle, hundreds of megabits/sec to major command posts, and kilobits/sec to the warfighters or individual tanks. Interactive wargaming simulations involving 100K nodes; remote medical services; information pull from 5 year on line archives; real time planning cycles. Global Grid concepts involve fiber where available, communications satellites, high flying RPV's, AWACS, Joint Stars, all operating together. Wireless LAN and wireless cellular technologies will be needed, with data flow control technologies to guide and link the data. Some LPI radios need to execute a FFT for each incoming data sample, requiring 200-300 million arithmetic operations/sec for 2.4 kilobits/sec. Communications cards already exist for workstations which can handle 155 megabits/sec on a fiber, with 622 megabits/sec shortly. Many or most of these systems will be mixed mode, combining analog and digital chips in the same subsystems.

The civilian telecommunications industry is trying to replace "circuit switched" paths with packet switched paths, since when the virtual circuit is quiet, no path has to be maintained, as would be the case for the circuit

switched paths. Radio links for wireless telecommunications are the fastest growing part of the civilian market. MCM-C, MCM-D, and MCM-L forms of multichip modules all have roles to play in the next generation of electronics for this field. Bare die will be used for wireless and line card applications, with flip chip attachment used rather than wire bonding connection approaches.

State of The Art of MCM Fabrication Technology for Mixed Mode Applications

The Hughes representative presented their metal organic MCM-D technology; it is clear that the Hughes MCM-D process is one of as many as eight metal layers, can have stacked ("coffee cup") vias, and has a wide range of control of dielectric thicknesses and layer stackups. Hughes is experimenting with the incorporation of spiral inductors and integral capacitors into their structure. Their vias have very shallow sidewalls, because they understood the vertical stress problems in the polymers. The shallow sidewalls prevent stress cracking. Hughes is building the MCMs for the F-22, and need to prepare MCMs in very large sheets, up to 12" x 12" inches or even larger, to decrease costs; they believe that such an approach will be feasible. Their designers see a wide variety of uses for all-digital, all- analog, and mixed mode modules, over a range of frequencies from the tens of KHz to many MHz.

The General Electric representative described their "chips-first" MCM technology, which by now has been so frequently discussed that we will not cover it further here. This process has been licensed to TI, who is developing a production facility for chips-first MCMs. A number of GE-internal needs for microwave, digital, and mixed mode MCMs have been identified. One mixed mode application of interest was not at all high speed, but very critical: for Full Authority Digital Engine Controls (FADEC) for jet aircraft engines produced by GE; clock rates and bandwidths are in the tens of KHz, but the application represents a critical technology.

State of The Art of Materials Technologies for Mixed Mode Applications

Dr. Eric Cross, Penn State Materials Research Labs and DSRC member: The state of the art of high permittivity dielectrics: Such materials are of interest to the capacitor manufacturing community, as well as possibly to the MCM community. Dielectric technology is still improving. For example, dielectrics are

being made much thinner; dielectric layers 1 micron thick are in research and development for discrete capacitors, with 7.5 micron thickness in production by the Japanese. This material is used for stacked capacitors for discretes. Thinner layers result in higher voltage breakdown strength, because avalanche problems are defeated. Lead zirconate titanate (PZT) does not loose its ferroelectric properties even in very thin layers. Barium Titante can be deposited in thin layers, but looses its ferroelectric properties in thin layers, dropping to K values of less than 1000. Conversely, PZT retains its ferroelectric properties down to 400 Angstrom layer thicknesses. Voltage gradients of 1.5-4 megavolts/cm can be established in PZT type films without breakdown.

Relaxor ferroelectrics have even better energy storage capabilities than do the ferroelectrics. The antiferroelectrics demonstrate an even larger energy storage capacity than either ferroelectrics or relaxor ferroelectrics. Some of these materials can in a sense flip back and forth between being ferroelectric AND antiferroelectric. Ferroelectric switching has been measured at 2.3 nsec; the same data is not yet available for antiferroelectrics. These materials, particularly the relaxors and the anti ferroelectrics, have much farther to go in terms of their development, and show great promise for improved discrete capacitors and especially, in very thin films, for integral capacitors in MCMs.

Dr. Paul Kohl, Georgia Tech: Metal Issues for advanced MCMs: Many materials such as copper or aluminum, other than silver, tend to loose their conductivity, from 95%, to 90%, and even down to 50-60%, in as-deposited form in comparison to their bulk properties, as a result of the deposition processes themselves. Silver does not loose its conductivity through process steps. Electroplated silver has a bulk conductivity and sheet resistance identical to the bulk material; this is not true for other metals. The principal problem with silver is the evolution of corrosion due to environmental of sulphides, not oxides. Stress is less in silver than in copper, Al, or gold, both during heating and cooling, because the silver plastically deforms, relieving stress. The cost of silver is $.50-1.00/inch2 of MCM surface area.

The cost of gold in an MCM is approximately $1 per inch2 of MCM area. However, even this cost is not really as high as it appears, because some processing steps can be skipped when gold is used; further, gold has an excellent shelf life. Silver is much less expensive than gold; the cost of the silver is vanishingly small in an MCM. A flash of gold on a silver upper layer could be applied in an MCM, but gold diffuses into silver. Further, it is not presently known how

much gold would be necessary to prevent corrosion, or whether the thin gold flash would affect the silver conductivity.

Dielectrics: Benzocyclobutane (BCB) can cure in 6 seconds, rather than the 2-3 hours required to cure the polyimides, which could be a significant manufacturing advantage. However, BCB cures with good planarization but with fairly high stress (these two go hand in hand); this high stress limits the number of layers which can be achieved with BCB. Thus, use of BCB is a mixed bag; some features are improved in comparison to polyimides, while some are worse. There are other organic formulations which might be even better than BCB or the polyimides, but little specific work has been done to identify them.

MIXED MODE ELECTRONIC PACKAGING

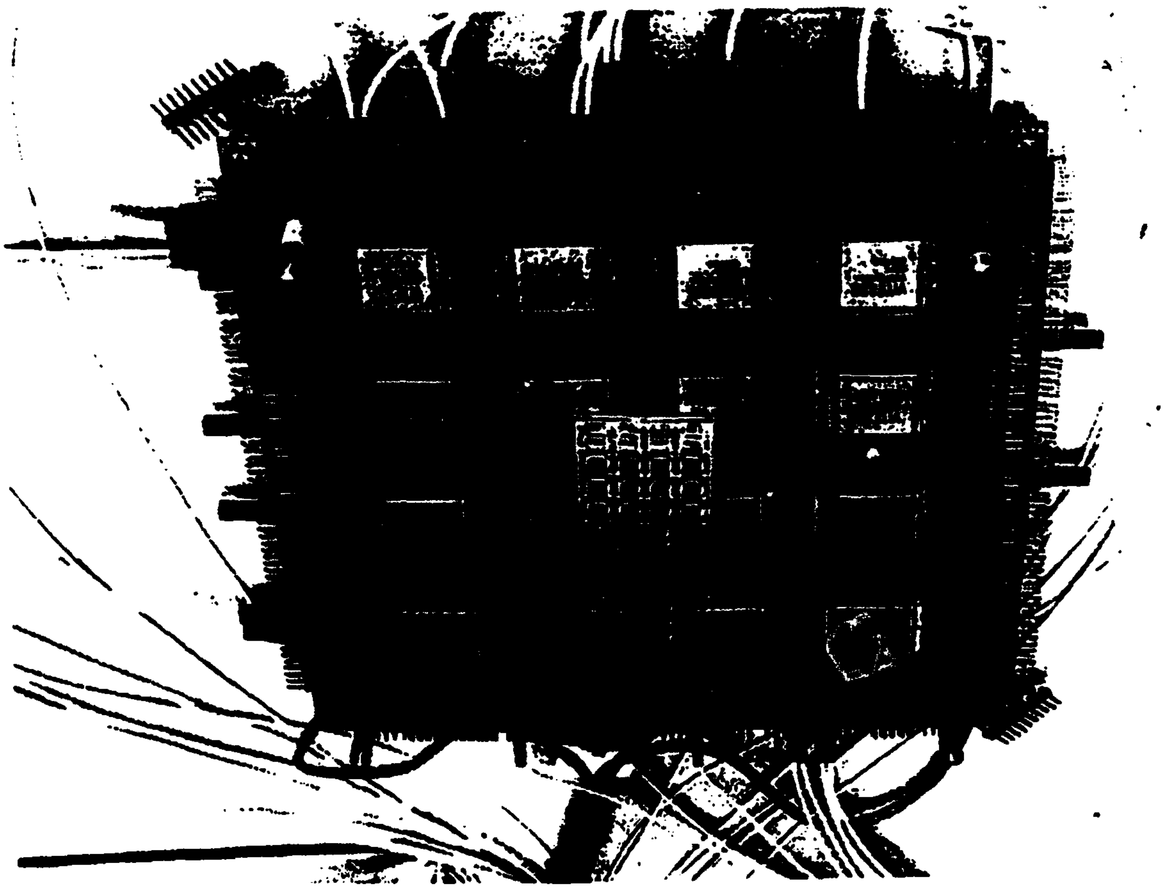
B. K. Gilbert and E. Cross

MILITARY APPLICATIONS FOR HIGH PERFORMANCE MIXED MODE ELECTRONICS

- Military radar (e.g., Air Force Digital X-band radar)
- Electronic warfare (ECM, ECCM, ESM)
- Wireless communications
- Wideband SONET Fiber Land Line Communications
- All-Digital baseband-switched communications satellites (e.g., Milstar Block 3)
- Many others, some only now being recognized

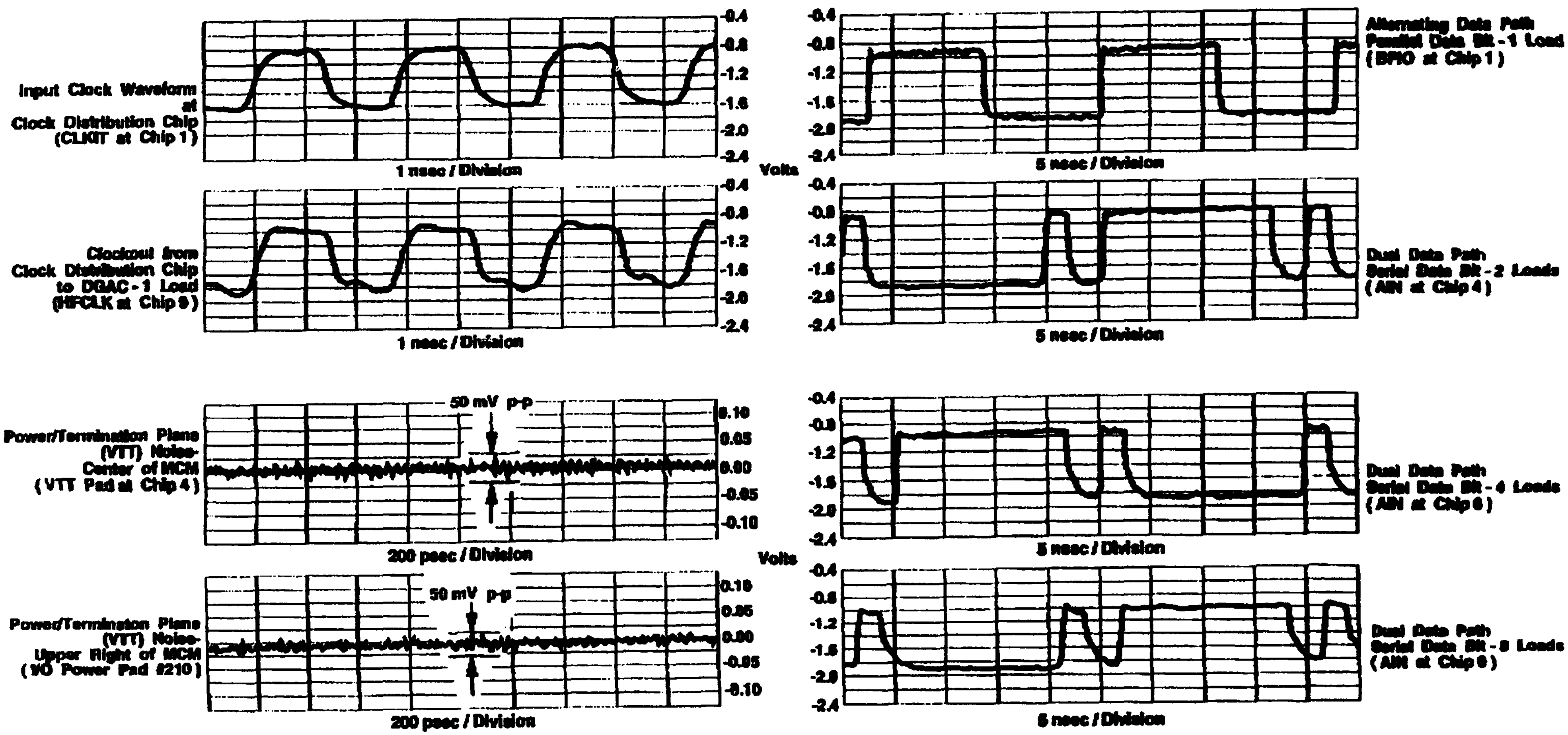
COMMERCIAL APPLICATIONS FOR HIGH PERFORMANCE MIXED MODE ELECTRONICS

- Radar detectors
- Automobile collision avoidance systems
- Test equipment
- Cellular, cordless, and visual telephones
- TV tuners
- Personal communication networks (PCNs)
- Wireless LANs
- Head and tail end circuits for fiber optics LANs and WANs
- All-Digital baseband-switched communications satellites (e.g., ACTS)
- Civilian Digital aircraft radar (airborne and ground based)



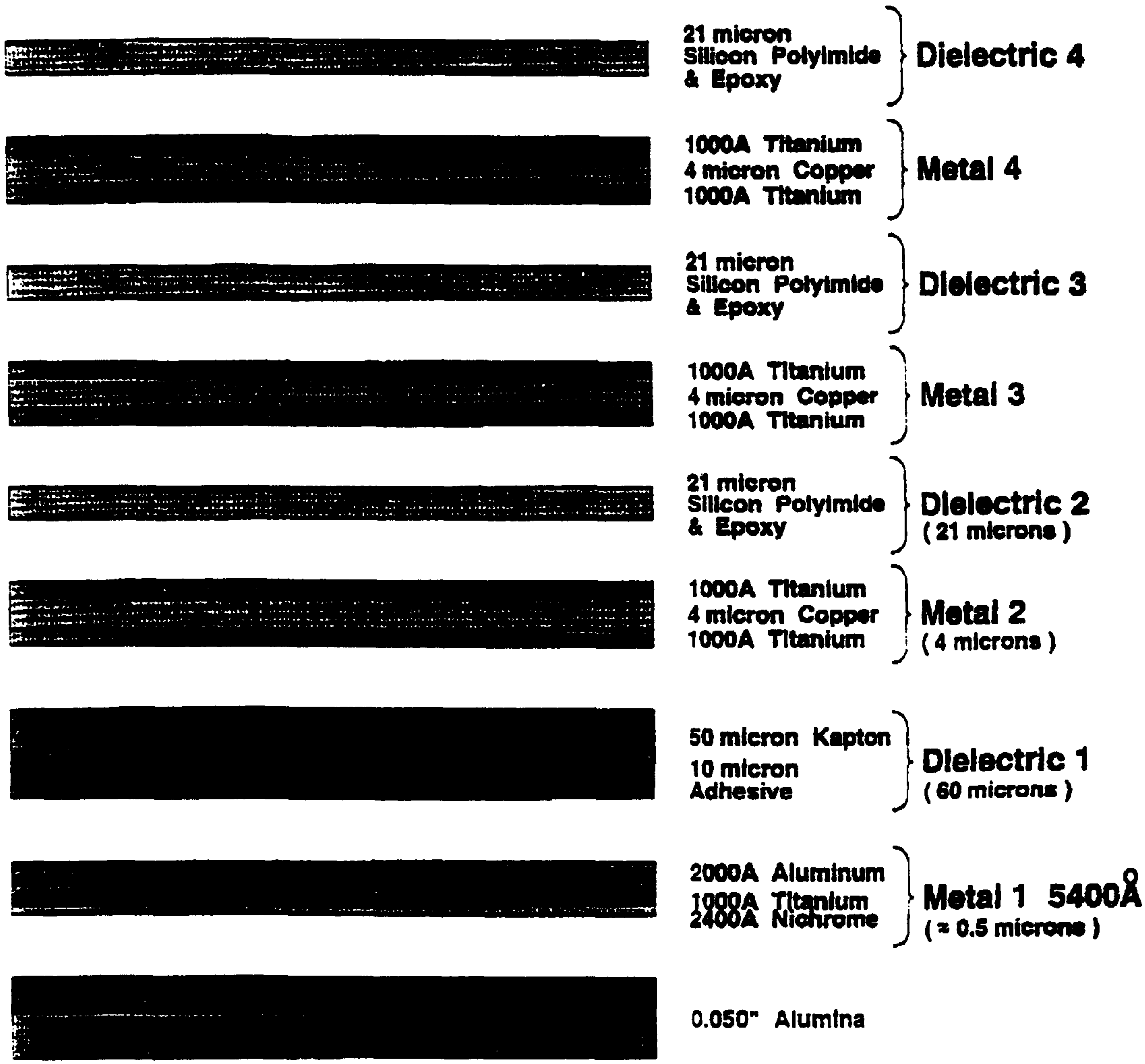
CLOCK, DATA AND POWER PLANE MEASUREMENTS TAKEN AT SELECTED INTERNAL LOCATIONS ON nCHIP SIXTEEN CHIP DEMONSTRATION MULTICHIP MODULE (TDV-3W)

(Mayo Standard Sixteen Chip Implementation Utilizing Vitesse VSC2K GaAs Gate Arrays [15 DGAC, 1 CLKDST]; Module Serial Number MCM1; "Chips-Last" Wire Bond Version; Discrete Decoupling Capacitors Added; All Signal Lines = 50 Ohm Shunt Terminated; Tested with Tektronix 11801A Oscilloscope, HP 8000/E2902A Clock/Pattern Generator, Mayo MCM Test Fixture, GGB Industries Pico Probes for Internal Measurements; 350 MHz System Clock Rate)



04 / 93 / DJS / 11467

DETAILED CROSS SECTIONAL VIEW OF TYPICAL COPPER-POLYIMIDE MULTICHIP MODULE



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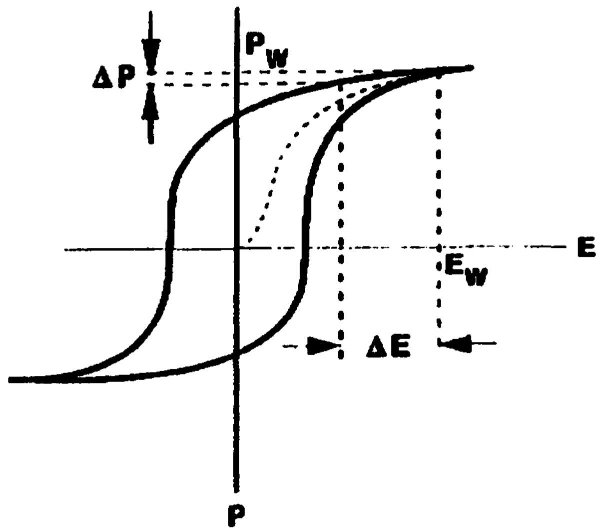
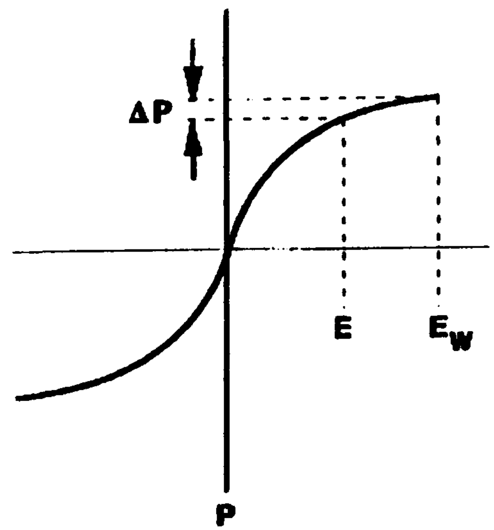
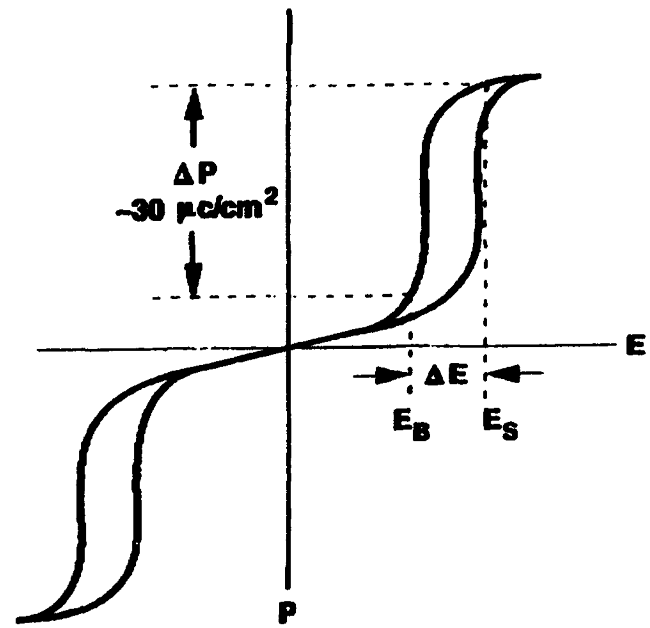
TYPICAL RESPONSES OF DIELECTRIC MATERIALS UNDER EVALUATION FOR USE AS AN INTEGRAL DECOUPLING CAPACITOR IN MULTICHIP MODULES



FERROELECTRIC



RELAXOR DIELECTRIC



ANTI-FERROELECTRIC

WHERE: P = Charge per Unit Area
E = Applied Field (Voltage)

04 / 93 / KJC / 11461

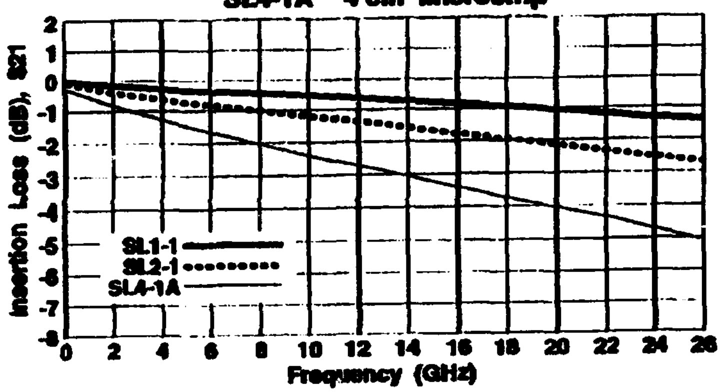
F6

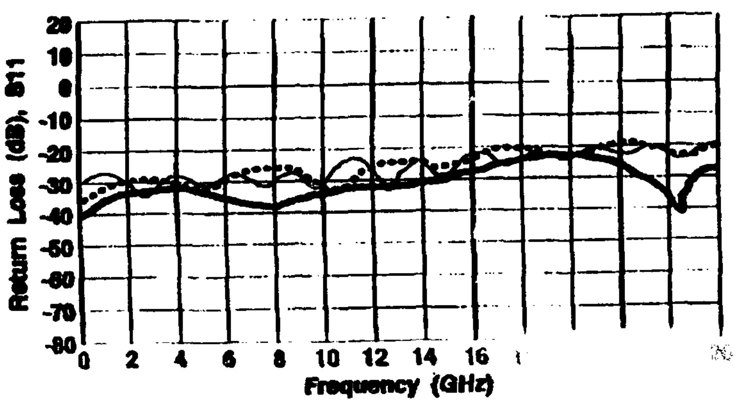
INSERTION AND RETURN LOSS . IGTH COMPARISONS OF 50 OHM MICROSTRIP AND STRIPLINE TRANSMISSION LINE STRUCTURES FABRICATED ON INTEGRATED SYSTEMS ASSEMBLIES (ISA) "CHIPS-FIRST" ADVANCED MULTICHIP MODULE PROCESS (AMCM)

(Mayo Standard Passive Coupon Design 01, Revision 0; 1993 Fabrication Run; Substrate Serial Number ISA1; 4 Metal Layers; Copper Metalization; Polyimide Dielectric; Line Width Thickness = 6 μm; Measured on HP 8510C Vector Network Analyzer with Cascade WPH-105-250 Microwave Probes)

Microstrip Structures, Line Widths = 75 μm

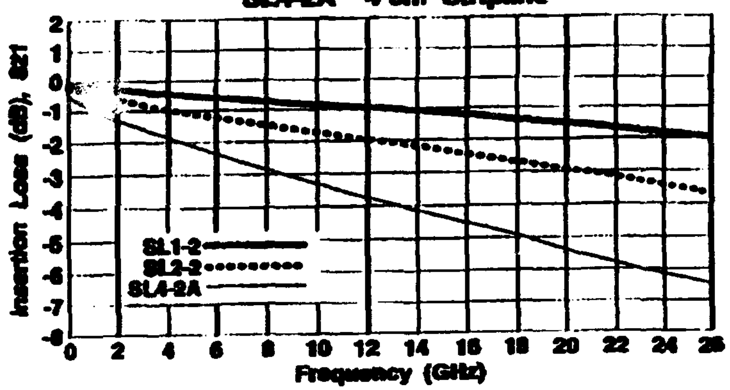
SL1-1 1 cm Microstrip
SL2-1 2 cm Microstrip
SL4-1A 4 cm Microstrip

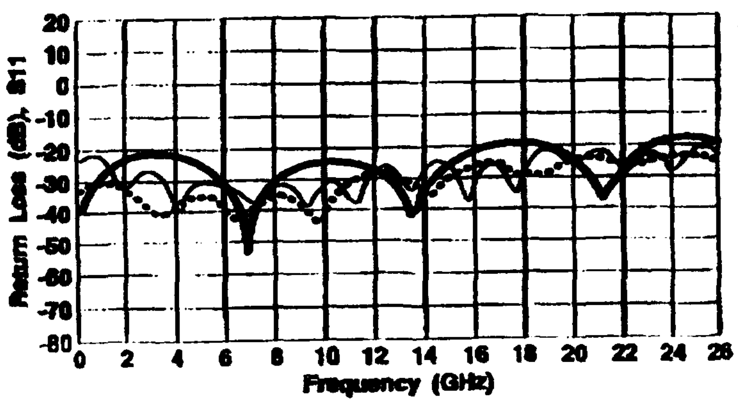




Stripline Structures, Line Widths = 34 μm

SL1-2 1 cm Stripline
SL2-2 2 cm Stripline
SL4-2A 4 cm Stripline





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F7

SOLUTION OF THE MIXED MODE PACKAGING PROBLEM - 1

- Improve as-deposited copper metallurgy
- Explore silver/gold metallurgy
- Improve lithographic definition of metal interconnects
- Develop low-K organic dielectric for better shielding and faster signal propagation

F8

SOLUTION OF THE MIXED MODE PACKAGING PROBLEM - 2

- Develop very high-K inorganic dielectrics for local storage of charge and decoupling
- Develop improved fabrication of integral deposited resistors/capacitors with low reactances
- Develop techniques for fabrication of integral inductors
- Develop techniques for on-MCM electromagnetic shielding and isolation of analog and digital components to -80 db

F9

SOLUTION OF THE MIXED MODE PACKAGING PROBLEM - 3

- Develop advanced electromagnetic modeling tools at 10-50 GHz
- Develop an Integrated Mixed Mode ECAD Tool Suite

F10

CREATE A "DEMAND-PULL FOR ADVANCED ELECTRONIC PACKAGING THROUGH INSERTION PROJECTS

- Develop initial demonstration "test coupons" containing passive structures and active chips, as proof of concept
- Develop a series of true MCM insertion projects

F11

MIXED MODE ELECTRONIC PACKAGING

Workshop Coordinator: Barry K. Gilbert

July 8, 1993

8:15 am	Introduction, Dr. Barry K. Gilbert (DSRC/Mayo Foundation)
8:20 am	"The Air Force Digital X-Band Radar Program", Franklin D. Lamb (Acting Branch Chief, Microwave Systems Technology Branch, Microwave Division, Solid State Electronics Division, Air Force Wright Laboratories)
9:00 am	"U. S. Government Need for High Speed Encrypted Communications and the Accompanying Need for High Performance Mixed Mode Systems and Electronic Packaging", Dr. William Semancik (Senior Electronics Engineer, Group R22, National Security Agency)
9:45 am	Break
10:00 am	"An Overview of Problems and Successes in MCM Technology, and the Features Required for Mixed Mode Electronic Packaging", Dr. Barry K. Gilbert (DSRC/Mayo Foundation)
10:40 am	"Raytheon Efforts in Mixed Mode Systems Operating at High Clock Rates", Dr. Behshad Baseghi (Ratheon Electromagnetic Systems Division)
11:20 am	"Civilian Telecom Applications at High Clock Rates and High Frequencies", Mr. John Pittman (Northern Telecom)
12:00 Noon	Lunch
1:00 pm	"Military Radar Applications for Mixed Mode Electronics; Design and Fabrication of Mixed Mode MCMs", Mr. Mike Gdula (General Electric Corporate Research and Development Center)
1:40 pm	"Dielectrics, Especially Ferroelectrics, for Advanced MCMs", Dr. Eric Cross (DSRC/Materials Research Laboratory, Pennsylvania State University)
2:20 pm	"Metallurgy Issues for Advanced Mixed Mode Electronic Packaging", Dr. Paul Kohl (Georgia Institute of Technology)
3:00 pm	"Mixed Mode MCM Design and Fabrication for the F-22 Fighter; Mixed Mode MCM Design and Fabrication Issues", Mr. Phil Trask (Hughes Aircraft Corp.)
3:40 pm	Open Discussions Begin

MIXED MODE ELECTRONIC PACKAGING

July 8, 1993

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MURPHY, James	ARPA/ESTO	703-696-2250
TRASK, Phil	Hughes Aircraft Co.	714-759-2520
WHITESIDES, George	DSRC/Harvard	617-495-9430

LIGHT EMITTING ORGANICS FOR VISIBLE DISPLAYS

Mark S. Wrighton and Henry Ehrenreich

EXECUTIVE SUMMARY

Workshop Objective

The purpose of the workshop on organic electroluminescence was to review the field with the aim of determining the viability of practical applications, especially displays. Special emphasis was placed on recent developments related to conducting polymers. Organic materials have long been known to exhibit electroluminescence, with significant work done in the late 1960's on single crystal anthracene. Recently, several groups have reported electroluminescent devices using conducting polymers as the light emitting materials. The workshop brought together the discoverers of electroluminescence in conducting polymers (Drs. Richard Friend and Alan Heeger) along with the leading experts [illegible]rganic electrogenerated chemiluminescence (Dr. Allen Bard) and organi[illegible]troluminescence (Drs. Ron Moon and Ching Tang). Key issues include fundamental factors affecting efficiency, durability, and manufacturability, and comparison of cost/performance with competing technologies. Significant industry participation among the speakers added enormously to the discussion of applications.

Relevance to DoD

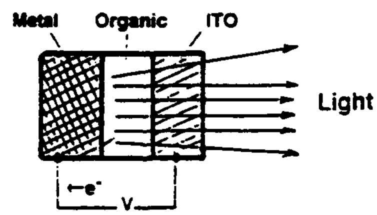
Displays are common in military systems, from aircraft to computer terminals to portable devices. Full color, high contrast, and low power consumption are critical in many applications. Light emitting diodes (LED's) from inorganic semiconducting materials have been important in small displays (e.g. calculators) but are regarded as too expensive for large displays, and furthermore blue SiC LED's are not efficient. Electroluminescent organic materials

have been demonstrated to be relatively efficient for the generation of blue light. Recent reports of electroluminescent conducting polymers suggest the viability of durable, efficient, and manufacturable electroluminescent devices. The area of light emitting organics may have other applications of interest to DoD including use in disposable electronic devices and in lighting to replace light bulbs. From the DoD perspective it is important to establish the advantages and limitations of organic electroluminescent devices.

Scientific and Technical Summary

Organic materials have long been known to be electroluminescent, with good work on anthracene crystals dating back to the late 1960's. The essential device structure for the solid state devices consists of an emissive organic layer sandwiched between two metallic contacts, one which injects holes and the other which injects electrons, Figure 1. Electrochemical devices involving the oxidation and reduction of solution species leading to the creation of

Figure 1
Organic LED



emissive excited states in electrolyte media could, in principle, be solid state, but most studies of the electrochemical devices have involved liquid electrolyte media. Several classes of organic materials have been studied, and considerable effort has been expended in academic and industrial laboratories to understand and optimize organic electroluminescent materials and devices. Below are given the major classes of organic electroluminescent materials, and Figure 2 illustrates examples of electroluminescent materials.

Classes of Organic EL Materials:

1. **Crystals**- e.g. anthracene; efficient, but expensive and fragile.
2. **Molecular Films**- e.g. metal oxinates; efficient, easy to prepare, but

are possibly not durable above 80 °C.

3. **Pure Polymers-** e.g. polyphenylenevinylene; new materials, properties not yet completely understood.
4. **"Doped" Polymers-** e.g. polyvinylcarbazole/polyphenylene vinylene; must be used at or near breakdown voltages.
5. **Molecules in Electrolyte Media-** e.g. 9,10-diphenylanthracene in CH_3CN/electrolyte; perhaps most efficient of all organic EL systems, but durability not demonstrated; there are manufacturing problems.

Electrochemical devices for generating electroluminescence demonstrate very efficient generation of excited state molecules in solution. Indeed, it appears that for every electron passed in the external circuit it is possible to create one excited molecule in a singlet emissive state. In certain cases where the photoluminescence quantum yield is near unity it is therefore possible to envision a device where one electron yields one photon, but such a device has not yet been unambiguously demonstrated. Nonetheless, there appears to be evidence to suggest that exceptional efficiency is possible in such devices.

While many solid state organic devices can be demonstrated to function in the simple mode represented in Figure 1, the most efficient systems involve the use of a heterojunction device as illustrated in Figure 3.

Figure 2

Organic EL Materials

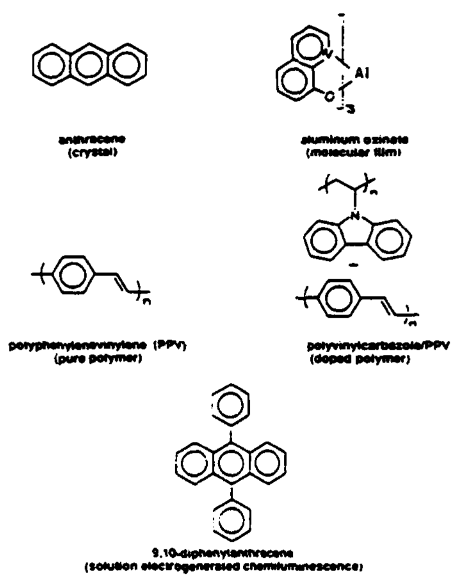
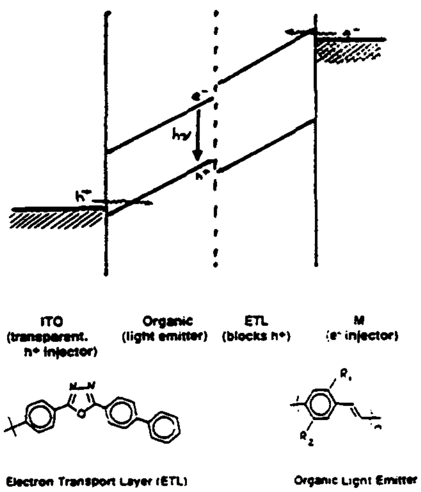


Figure3

Heterojunction Solid State Organic LED



The key is that the electron transport layer blocks hole transport and radiative electron-hole combination occurs near the junction of the two organic layers. It is important to note that on-off times and brightness are regarded as acceptable for display applications. In particular, efficiency of blue organic LED's (1% yield of photons/electron) significantly exceeds that of inorganic semiconductor devices, e.g. SiC (0.1% yield of photons/electron). Cost and manufacturability have not been well established for organic LED's, but there appear to be viable and major practical applications, based on input from both Kodak (Dr. Ching Tang) and Hewlett-Packard (Dr. Ron Moon).

The following critical issues have been identified as ones deserving further consideration:

Degradation of Organic EL Materials

All organic materials have questionable lifetime at high current density and at temperatures associated with processing of semiconductors. Most agree that >10,000 hr. lifetimes are needed. At this point at least some 2000 hr. tests have been done, but the devices show much more degradation than do inorganic semiconductor LED's. However, little effort has been expended to establish products of degradation, mechanisms of degradation and methods to suppress degradation in organic EL devices. Organic films of some of the most efficient EL molecules may not be durable above about 80 °C, owing to intrinsic properties. Polymers can be expected to be durable above this temperature, but significant tests have not been done.

Reactive Metal Contacts

Recent experiments with new organic EL materials involve the use of reactive metals as the electron injection contact, e.g. Ca, Mg, or Al. These materials require protection from the atmosphere (O_2, H_2O, etc.), in order to obtain durable devices. A critical question here is whether encapsulation will be effective. It is also interesting to speculate on whether the type of heterojunction devices shown in Figure 3 will allow the use of a less

reactive metal contact. While this may be possible, the problem of increased operating voltage (to overcome the large barrier to electron injection) requires attention.

Solid State vs. Solution Photoluminescence Quantum Yield

Molecules in solution have been demonstrated to exhibit very high photoluminescence quantum yields. However, pure solid films of the molecule typically exhibit significantly diminished photoluminescence quantum yields. The lower yield in the solid state is attributed to non-radiative impurity quenching of the excited states which migrate from molecule to molecule by well-established energy transfer mechanisms. Energy migration to a non-luminescent impurity suggests that purification will improve photon yield from excited species. There may be, however, other mechanisms for quenching that cannot be overcome by purification, e.g. excimer formation to yield a non-luminescent excited dimer. In any event, the yield of photons/electron in EL devices is apparently limited by low yields of photon emission from excited states compared to the excited states produced in fluid solution.

Spin Statistics and EL Efficiency

The prevailing view is that the theoretical efficiency of photons/electron in organic EL devices is 25%, based on the 1:3 statistical probability of forming the emissive singlet vs. the non-emissive triplet. This theoretical expectation may not be valid when the energetics for forming the singlet and triplet are different, owing to the fact that excess energy of the e^--h^+ pair must be converted into vibrational energy. This may lower the effectiveness of e^--h^+ encounters destined to form, say, a low energy (compared to the singlet excited state) triplet excited state. In any event, it may be possible to overcome the problem by designing molecules incorporating heavy elements such as d-block transition elements of the 2nd and 3rd row. Molecular complexes involving these elements can have very emissive lowest excited states having nominally spin-forbidden transitions; the spin-orbit coupling is sufficiently great that large radiative probabilities

can exist for such situations. It is perhaps most noteworthy that the yield, from two independent measurements, of photons/electron in the electrogenerated chemiluminescence from Ru(2,2'-bipyridine)$_3^{2+}$ is the same as the photoluminescence quantum yield from the lowest triplet excited state of the complex. There are two key points: the theoretical expectations from statistical arguments may not apply, and molecular engineering may overcome problems resulting from the creation of non-emissive excited states.

While there are serious obstacles to major applications of electroluminescent materials, it is evident that there has been significant progress. The following summarize the scientific and technological situation:

- Organic materials can be tailored rationally to achieve key properties such as color of emitted light, efficiency, durability, and processibility.
- Relatively high EL efficiency has already been achieved in solid state devices (1-2% yield of photons/electron) and studies of electrogenerated chemiluminescence in solution suggest efficiency can approach 100%. Some fundamental factors governing solid state efficiency are not fully understood.
- Operation at low voltage, typically <5 V, and frequency adequate for displays has been demonstrated.
- Degradation is a critical issue. Little work, however, has been done to apply modern organic chemistry knowledge and techniques to this problem area. Demonstrated lifetimes of organic EL devices (with about 50% decline in efficiency) of 2000 hr. have been reported.

Conclusions and Observations

The following are the essential conclusions and observations regarding organic EL materials and devices:

- Organic materials show genuine promise for use in EL devices, especially for blue light.
- In display applications, power needs, speed, and operating voltage of organic EL devices appear to be tolerable.

• Applications other than displays are possible, and there are suggestions that even lifetimes at 2000 hr. (or less) may be useful. At one extreme lighting systems (replacing light bulbs) are possible and disposable electronic devices and trinkets seem possible at the "low end".

• Theoretical limitations to efficiency are not well established and results from electrogenerated chemiluminescence suggest that efficiency of photons/electron could approach 100%.

• Mechanisms of degradation and methods for improving lifetime need to established.

• New materials and new combinations of materials should continue to be explored. Examples would include polymer analogs of molecular films, "composites" of solid state polyelectrolyte/conducting polymers, and 5d transition element-containing polymers. It is premature to settle on one materials system for any application.

• There is little information on cost or manufacturability, but cost/performance would appear to be very competitive with conventional LED's for some major applications, particularly blue LED's.

LIGHT EMITTING ORGANICS FOR VISIBLE DISPLAYS

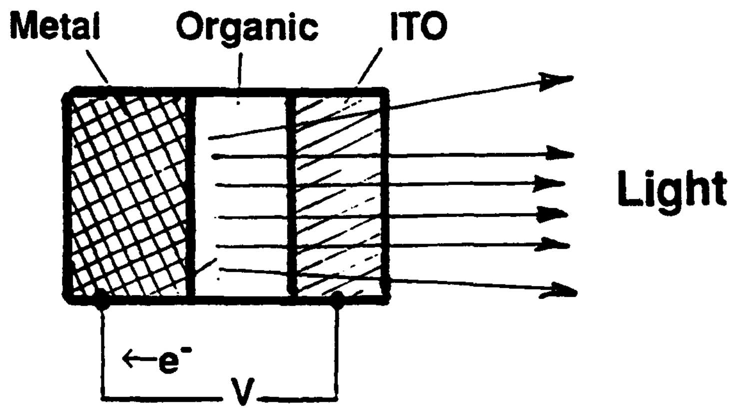
Mark S. Wrighton and
H. Ehrenreich

Objective and DoD Relevance

<u>Objective:</u> Assess organic materials for use in electroluminescent devices for display applications. Key issues include fundamental factors affecting efficiency, durability, manufacturability, and comparison of cost/performance with competing technologies.

<u>DoD Relevance:</u> Many DoD systems use active display devices. Full color, high contrast, and low power are critical in many applications. Recent research has shown that new conducting polymers may be useful in electroluminescent devices: what advantages do these devices have for DoD uses and what are their limitations?

<u>EL Device:</u> Application of potential results in current flow and emission of light from the organic.



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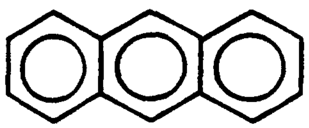
Pure Polymers- e.g. polyphenylenevinylene; new materials, properties not yet completely understood.

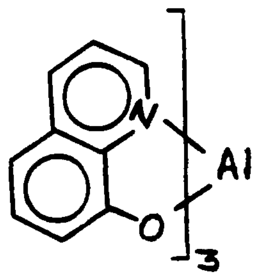
"Doped" Polymers- e.g. polyvinyl-carbazole/polypheneylenevinylene; must be used at near breakdown voltages.

Molecules in Electrolyte Media- e.g. diphenylanthracene in CH_3CN/electrolyte; perhaps most efficient, but durability not demonstrated; manufacturing problems?

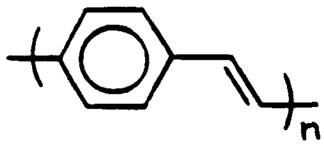
Organic EL Materials



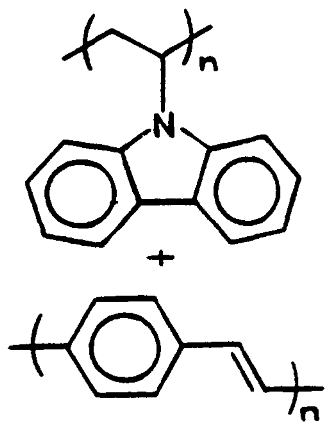
anthracene
(crystal)



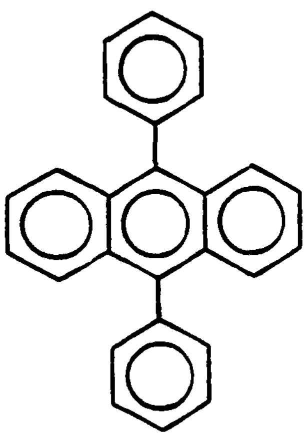
aluminum oxinate
(molecular film)



polyphenylenevinylene (PPV)
(pure polymer)

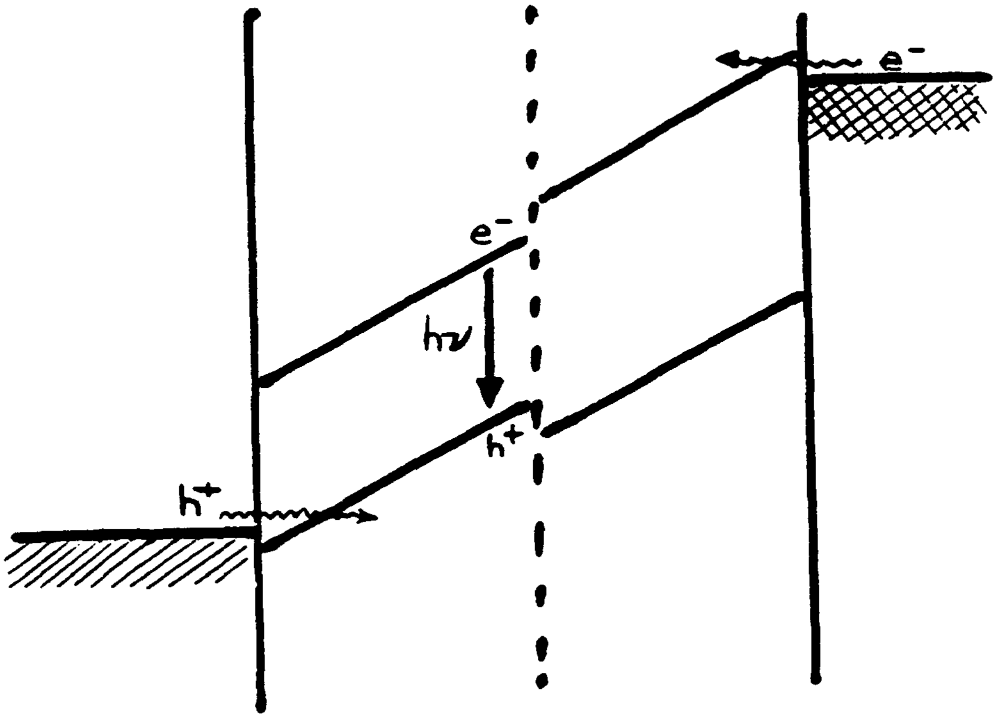


polyvinylcarbazole/PPV
(doped polymer)

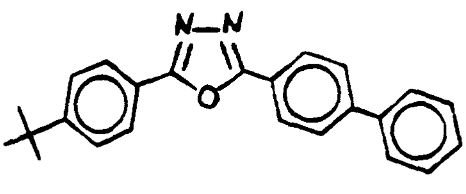


9,10-diphenylanthracene
(solution electrogenerated chemiluminescence)

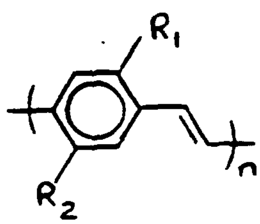
Heterojunction Solid State Organic LED



ITO (transparent, h+ injector) | Organic (light emitter) | ETL (blocks h+) | M (e- injector)



Electron Transport Layer (ETL)



Organic Light Emitter

Critical Issues

Degradation of Organic EL Material

All organic materials have questionable lifetime at high current density and at temperatures associated with processing. Most agree that >10,000 hr. lifetimes are needed. Can mechanisms of degradation be established by modern organic chemistry techniques?

Reactive Metal Contacts

Recent experiments with new materials use reactive metals such as Ca, Al, Mg as the electron injection contact. Can these be encapsulated? Will heterojunction organics allow use of more durable electron injection contacts?

Solid State vs. Solution Photoluminescence Quantum Yield

Molecules in solution exhibit very high luminescence quantum yields, but in the solid state these yields are much lower (presumably due to impurities quenching the excitons). Is the quenching mechanism in the solid state correct? Can purification yield higher photoluminescence yields resulting in higher EL efficiency?

"Spin" Argument and EL Efficiency

The prevailing view is that theoretical efficiency of photons per electron is limited to 25% due to the probability of forming the emissive singlet vs. the non-emissive triplet state of the organic. Is this view correct? Can emissive triplets be formed by using molecular engineering?

Electroluminescent Organics

• Organic materials can be tailored for essential fundamental properties, color of emitted light, efficiency, durability, and processibility.

• Relatively high EL efficiency has already been achieved, especially for blue light; photons/electron=0.01!

• Degradation is a critical issue. Little work has been done to establish mechanisms of degradation, but "tests" have shown >2000 hr. lifetime is possible.

• Fundamental factors limiting efficiency are recognized, but not fully understood; ~100% photon/electron yield is possible.

• Operation at low voltage, <5 V, is typical.

Conclusions

- Organic materials show genuine promise for use in EL devices, especially for blue light.

- In display applications power demands would appear to be tolerable.

- Applications other than for displays are possible, and there are suggestions that even lifetimes at 2000 hr. (or less) may be useful. Opportunity may exist for lighting applications at one extreme and for disposable devices and trinkets at the "low end".

- Theoretical limitations to efficiency are not well established; some evidence suggests nearly 100% efficiency (photon/electron) is possible.

- Mechanisms of degradation and methods for improving lifetime need to be established.

- New materials and new combinations of materials should be investigated; examples include polymer analogues of molecular films and composites of polyelectrolyte/conducting polymer systems. *It would be premature to settle on one materials system for any application.*

- Little information available on cost or manufacturability, but cost/performance would appear to be very competitive with conventional LED's for major applications, particularly blue LED.

LIGHT EMITTING ORGANICS FOR VISIBLE DISPLAYS

Workshop Organizer: Henry Ehrenreich
Chairman/Workshop Organizer: Mark S. Wrighton

July 9, 1993

8:00 am	ARPA Perspective, D. Slobodin (ARPA)
8:30 am	"Light Emission from Conjugated Polymers; Photoluminescence in Light Emitting Diodes: Progress and Promise", A. J. Heeger (UCSB)
9:30 am	"Light Emitting Diodes Based on Conjugated Polymers", R. H. Friend (Cavendish, Cambridge)
10:30 am	Break
11:00 am	"Electrogenerated Chemiluminescent Systems", A. J. Bard (University of Texas, Austin)
12:00 Noon	Lunch
1:00 pm	"Progress in Vapor Deposited Organic Electroluminescent Devices", C. W. Tang (Eastman-Kodak)
2:00 pm	"Can Polymer LEDs Compete?", R. L. Moon (Hewlett-Packard)
3:00 pm	Discussion and Summary
4:00 pm	Adjourn

LIGHT EMITTING ORGANICS FOR VISIBLE DISPLAY

JULY 9, 1993

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STATISTICAL LIMITS OF ULTRA-SMALL DEVICES

D. K. Ferry, M. Beasley, E. Hu,
T. C. McGill, and R. Osgood

Objective of Workshop

The level of increase of density in integrated circuits is continuing to maintain its progression, with a factor of 4X increase in chip density occuring every three years. As a result, devices are becoming smaller in each successive generation. For some years, it has been believed that statistical fluctuations in doping concentrations, interface smoothness, and oxide leakage would limit the extent to which continued shrinkage in size could continue. Device design and fabrication has undergone significant change in the period since these first predictions were presented, and many effects have been ameliorated by changes in device design, so that it was decided to hold a workshop to reassess the impact that statistical fluctuations would have on devices in ensuing generations. Representatives from major industrial organizations and leading researchers were brought together to discuss the various aspects in which these fluctuations could impact future performance. Speakers were asked to:

- Discuss the type of fluctuations they were experiencing and the manner in which these fluctuations arise, as well as how they are thought to impact devices performance.
- Provide a background of relevant theoretical and experimental work supporting their views, as well as predict the future scale of such fluctuations in devices.
- Were there architectural techniques to reduce the effects of fluctuations?

DoD Relevance

Modern microelectronic integrated circuits, and *systems*, are crucial to performance of modern smart weapons systems, to communications, as well as to command and control support systems. Continued evolution of growth in integrated system density will allow continued improvements in overall system preformance. As the size of the effective military force is reduced, it becomes

more important that DoD have the highest performance, highest-density electronic systems. Hence, the ability of the U.S. to control the continued integration density of high performance chips is a major defense objective. Further, large scale integration in electronic chips is one of the best examples of a dual-use technology. To push the ultimate limits is one goal of the current ARPA Ultra program, and it is necessary to continue to evaluate any and all possible processes which will impact the success of this latter program.

Scientific and Technological Summary

It is quite likely that continued evolution in semiconductor devices used in integrated circuits will provide dramatically reduced device sizes, down to at least 30 nm gate length, provided that (currently) secondary processes such as statistical fluctuations in device parameters do not become zero-order considerations and prove to be a "killer." The fabrication of the actual device in an integrated circuit involves multiple stages of dopant insertion, etching, oxide (or other insulator) growth, and thermal cycling. Each of these processes has the capability of providing significant deviations from the desired average resulting parameters (such as impurity concentrations, interface roughness, oxide thickness and resistivities, etc.). The statistical variations of the parameters from their nominal values is not usually a significant probl n devices today, primarily because device size is quite large on the average size scale of the fluctuation. However, in future devices this is not likely to remain the case. Even when "nominal" values are well controlled, the variance around these nominal values grows as devices become samll and the number of dopants, defects, etc., become small. The variation in device performance, due to the lack of a "nominal" value for many of the parameters, will begin to become important in future devices early in the next century. Whether this occurs in 2004 (at 0.12 mm design rules) or in 2020 (at 30 nm design rules, assuming only marginal slowing in the downscaling of design rules) depends crucially on whether a worst-case scenario or a best-case scenario is adopted. Unfortunately, there is insufficient knowledge about the effect of statistical fluctuations in real devices to be able to make a more definitive prediction of the problem timeframe.

Conclusions

The end of the evolution of integration density in microelectronic systems may well lie with processes other than the statistical fluctuations within

individual devices (such as with limitations in the availability or affordability of advanced lithography tools, which is discussed elsewhere, or with failures in advanced metallizations for these chips). However, if these problems are solved, as is likely to be the case, then evolution of the chips to design rules at the 0.1 mm and below will lead to a realm in which statistical fluctuations become zero-order effects in device performance.

The ARPA Ultra program addresses devices for ultra-fast, ultra-dense chips that are needed to reach future densities of 1 Tb on a single chip. Success of this program, with current device technology, will require the control and suppression of statistical fluctuations in order to achieve overall system performance. Or, alternatively, circuit approaches with high device characteristic variance will be required. However, studies of such statistical effects have been mainly laboratory investigations that have not addressed the effects in real-world-type devices. In most cases, the effect of statistical fluctuations on device performance is dependent upon the specific details of the device being studied, and no general scaling relationships are expected to be applicable. Moreover, these specific details can change in time, for example due to the motion of a single impurity (dopant) atom. Researchers tend to concentrate on their *typical best* results to show how good devices can be; here, efforts also need to focus on their *typical worst* devices to assess ranges of detrimental performance that can be traced to the effect of statistical fluctuations. The temporal stability of device characteristics, due to the temporal motion of impurities, also needs to be examined with more care.

Suggestions for Actions by ARPA

The continued progression of integrated circuits will lead to devices with effective gate lengths well under 0.1 mm within the next two decades. For continued progress, it is necessary to understand, and deal with, the role that statistical fluctuations in material parameters and transport parameters will play in device performance. This is as true for the large-foundary-produced ultra-large scale integrated circuits as it is for the single-wafer, cluster-tool-produced special purpose chips needed in small lot sizes. It is important that these effects be evaluated in a realistic device context.

• A large-scale program directed solely at studying statistical fluctuations is not warranted. Most of the effects of concern here are specific to the device structure, and do not appear to be generic in nature.

• An expansion of the Ultra program to allow studies of device-specific effects of statistical fluctuations would leverage both the Ultra program and its impact on future ULSI technology that is evolving from current device approaches. As part of the Ultra program currently underway within ARPA, research devices on the appropriate size scale are already projected for study.

• Studies of conventional semiconductor device scaling below 0.1 mm should also include considerations of statistical fluctuations.

APPENDIX

Introduction

Progression in the density of individual devices on an integrated circuit chip has followed a well-recognized scaling rule, in which the number of transistors has increased 4X each three years, while the design rule has decreased by 0.7X. This progression drives the technology, with DRAM being the leading edge chip, while random logic chips tend to follow about one generation behind. The leading edge requirement in resolution, or in design rule, as suggested by the Semiconductors Industry Association (SIA) is shown in Fig. 1. Following this progression, it is expected that we will reach 0.1 mm in 2007. On the other hand, careful evaluations by theoreticians in the U.S. and Japan, including recent work by Carver Mead, suggest that there is no conceptual problem in shrinking the Si MOSFET gate lengths (and design rules) to 0.03 mm, and perhaps slightly further. These considerations, however, assume that there are no statistical limits that will lead to fluctuations in device performance that prove to be "killers" of the device technology.

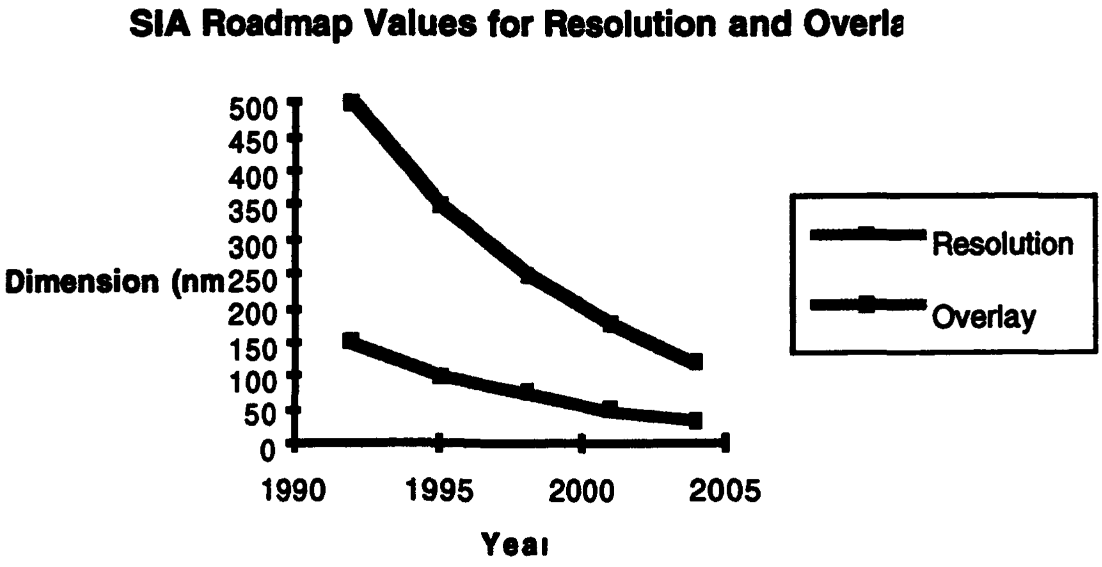

Figure 1

In contrast to this optimistic viewpoint, it was anticipated many years ago that statistical variation in the doping profile across an integrated circuit chip would lead to a device-to-device fluctuation in threshold voltage that

ultimately could limit the integration density. However, modern fabrication procedures routinely include careful channel implants of dopants to control the threshold voltage within acceptable limits, and such engineering procedures can be expected to be further developed to control such doping fluctuations *within some undetermined range.* That is, it may no longer be possible, at some future device size, to control all of the sources of fluctuation in device parameters to a sufficient level to allow continued evolution of the ULSI chip density.

The level of the problem can be pictured by noting that a typical future ultrasmall MOSFET may have a gate length of 0.05 mm and a gate width of 0.1 mm. If the channel density is 2×10^{12} cm^{-2}, then there are only 100 electrons under the gate. To achieve this inversion density at a gate bias of 1.6 V (expected in future ultrasmall devices), the gate oxide must be less than 4.5 nm thick. Lower voltages require correspondingly thinner oxides. Control of threshold voltage across any subsequent chip requires very tight control of processing parameters to achieve e.g. less than a monolayer variation in the average oxide thickness across the entire wafer. Even then, statistical variations due to defects in the oxide may need to be considered.

Sources of Fluctuations

The growth of thin (or thick) layers of materials in a controlled fashion depends upon basic chemical principles including interfacial reactions and the diffusion of various species. It is now becoming realized that the nonequilibrium process of film growth itself is a nonlinear process that, by its nature, produces roughness at the growth interface. This roughness increases with film thickness, so that the need in future ultrasmall devices for thinner films is likely to be a blessing. Moreover, the roughness incorporated by the growth process has many characteristic length scales, only some of which will have important consequences for device performance. There are several competing, and sometimes controversial, theories and regions of thin film growth. However, by their nonlinear nature, they often depend dramatically upon boundary (or initial) conditions, and therefore the results will be quite specific to the device structure in which the film growth is incorporated. The nature and consequences of such potential variations are not now understood.

The incorporation of dopants is also important, not only in the channel, but also for creation of controllable contact behavior. It is not, in general, desired to have the impurities ordered, as this leads to unwanted behavior, but random distributions lead to larger variances in the *local* density (as opposed to the *average* density) of impurity. It is known that many properties, such as contact resistance and breakdown field, depend in a detailed manner on the local density, with tunneling/breakdown currents flowing through the highest local field path. This is also true in leakage currents through oxide (and other insulator) films. Dramatic variances in tunneling currents can be expected if impurities or defects exist in the films, and this can lead to large device-to-device variance in both oxide leakage currents and turn-on behavior.

Lateral variations in device performance are incorporated usually through overlay errors in the lithography process. Variations in the actual gate length will lead to variations in the turn-on performance as well as to large variations in the actual drive current available from individual devices. It is not at all clear that current CAD tools used in circuit design have the latitude necessary to provide circuit and/or architectural solutions to the wide variation in device parameters that may arise from the above fluctuations.

Finally, the small number of charged impurities under the gate, and the short gate length lead to new sources of fluctuations, that are best described as quantum in nature. Quantum effects are characterized not only by the de Broglie wavelength of the carriers, but more importantly by the phase coherence length of the carriers (often called the energy relaxation length or the inelastic mean free path). This length (even in Si) can be more than 50 nm, even at room temperature, when the channel is on. Turning the channel on is another matter, and the electrons may move from source to drain via a percolation path—winding their way through the impurity potentials by a random walk. The long phase coherence length may lead to quantum interference between different electrons (recall there are only 100 of these at best), which produces conductivity modulation. At low temperatures, where it has been studied, this could be 40-50% of the actual drain conductance for a single interference path. This arises because the device is sensitive to the exact location of the impurities, and ensemble

averaging is beginning to break down. While the effect is reduced at higher temperatures, the temperature variation is quite weak, so that the effect may occur even at room temperature to a significant effect. The process is more complicated, as these interference paths may change with time, so that the fluctuations during one switching cycle may be quite different from those of another, or even during a single cycle.

Summary

While other processes, such as lithography, may ultimately limit the down-scaling of ULSI, the role of fluctuations within individual devices, whether these fluctuations are induced by fabrication or merely the small size, could well provide a limit. In any event, their effects will have to be considered. While fluctuations have been studied, the nonlinear manner in which these affect device performance precludes making assessments based upon such disjoint studies of fluctuations. In most cases, the effect of statistical fluctuations on device performance is dependent upon the critical details of the device being studied, and no general scaling relationships are expected to be applicable.

The ARPA Ultra program addresses devices for ultra-fast, ultra-dense chips that are needed to reach future densities of 1 Tb on a single chip. Success of this program, with current device technology, will require the control and suppression of statistical fluctuations in order to achieve overall system performance. However, studies of such effects have been mainly incidental laboratory investigations that have not addressed the effects in real-world-type devices for their own sake. Researchers tend to concentrate on their *typical best* results to show how good devices can be; here, efforts also need to focus on their *typical worst* devices to assess ranges of detrimental performance that can be traced to the effect of statistical fluctuations.

STATISTICAL LIMITS OF ULTRA-SMALL DEVICES

D. K. Ferry, M. Beasley, E. Hu,
T. C. McGill and R. Osgood

DS
RC

STATISTICAL LIMITS OF ULTRA-SMALL DEVICES

by

D. K. Ferry, M. Beasley, E. Hu, T. C. McGill, and R. Osgood

Objective:

To discuss the various aspects in which fluctuations in parameters of future ultra-small devices for ULSI could limit the effectiveness and utility of the devices.

DoD Relevance:

Modern microelectronic integrated circuits and systems are crucial to performance of smart weapons, communications, and command and control. ULSI is also a dual-use technology important to a large high technology electronics industry.

Defense Science Research Council *July 1993*

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Scientific and Technological Summary

- Continued evolution in integrated circuits will continue for the forseeable future. Device sizes may reach 30 nm gate length, but fluctuations may provide a limitation earlier.
- Variations in interface smoothness, small numbers of real dopants and defects, comparability of dimensions to critical quantum length scales, all will contribute to important effects which may provide hard limits to down-sizing.
- Most studies of fluctuations are not relevant to devices: effect of fluctuations on device performance are specific to the actual device under study—there does not appear to be a general scaling rule for these fluctuations.

J.T. WALLMARK, and S.M. MARCUS,
PROC. IRE 50, 286 (MARCH 1962).

J.T. WALLMARK,
in MICROELECTRONICS, Edited by E. KEONJIAN,
(MC GRAW-HILL, NEW YORK, 1963), CH. 2.

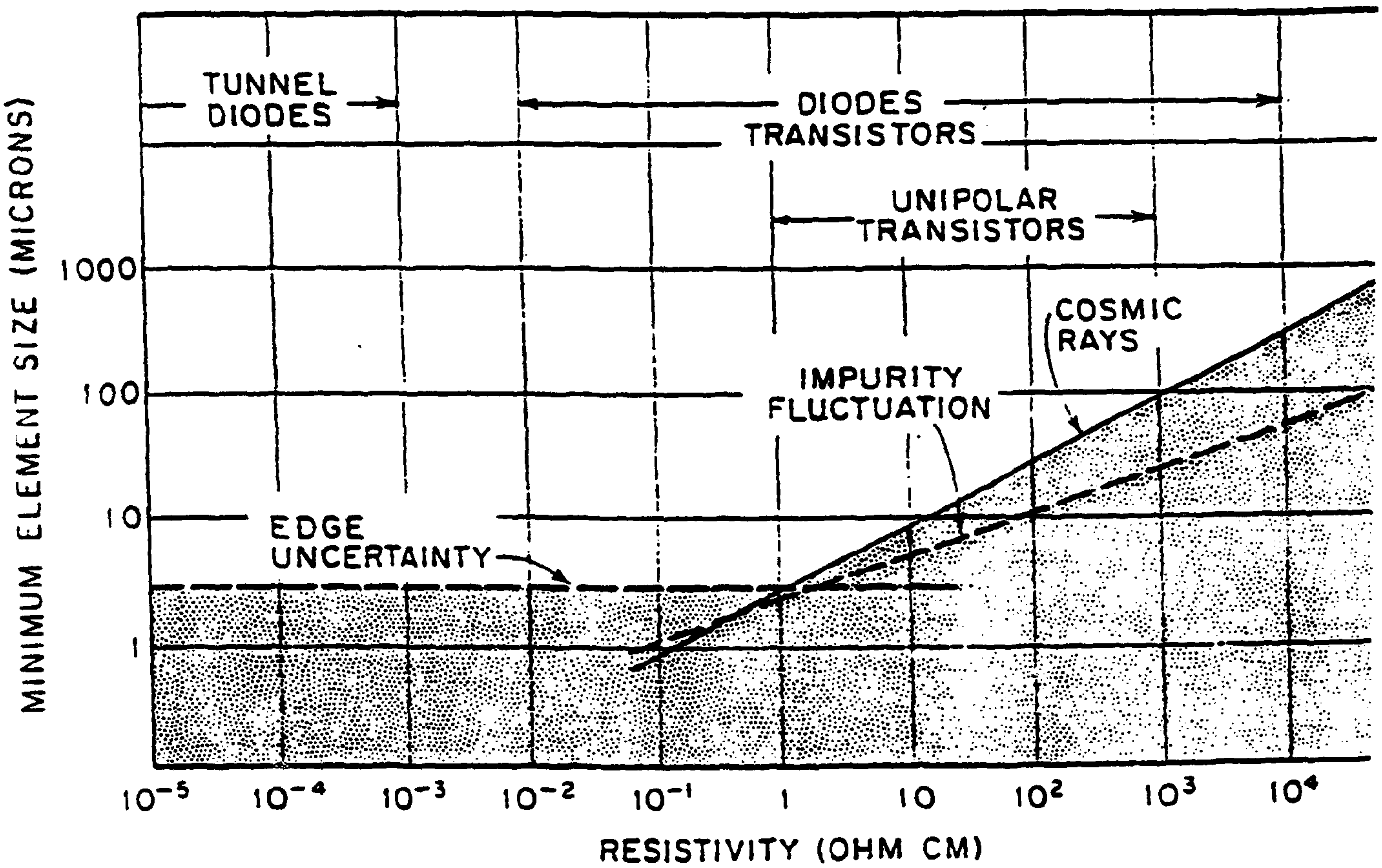
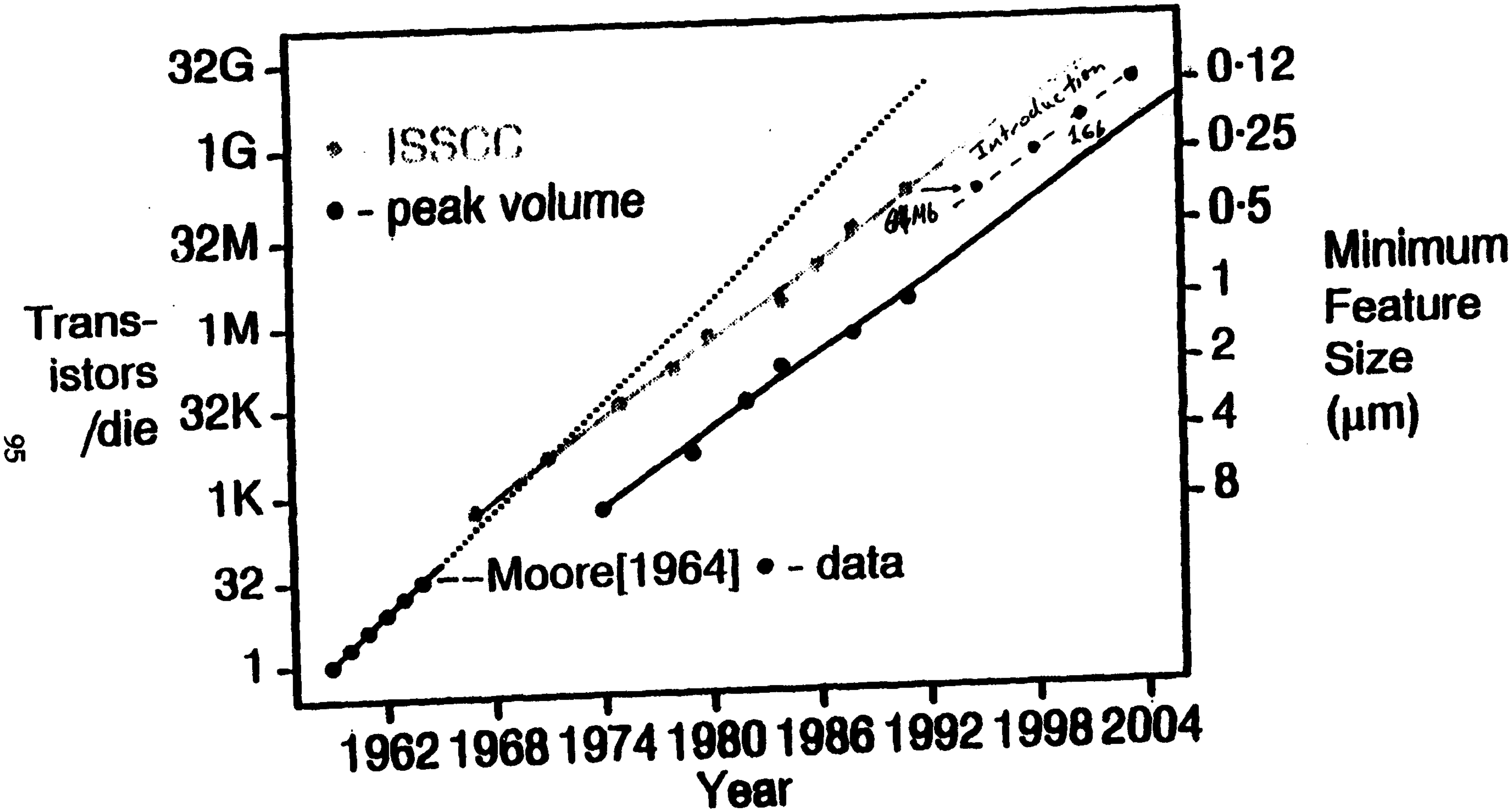


FIG. 2-3. Minimum device size versus resistivity of the material. Common : for some devices are indicated. Gray area is excluded.

1969: 1μ SCHOTTKY BARRIER TRANSISTORS

1988: .07μ CHANNEL LENGTH IN FET

Moore's plot



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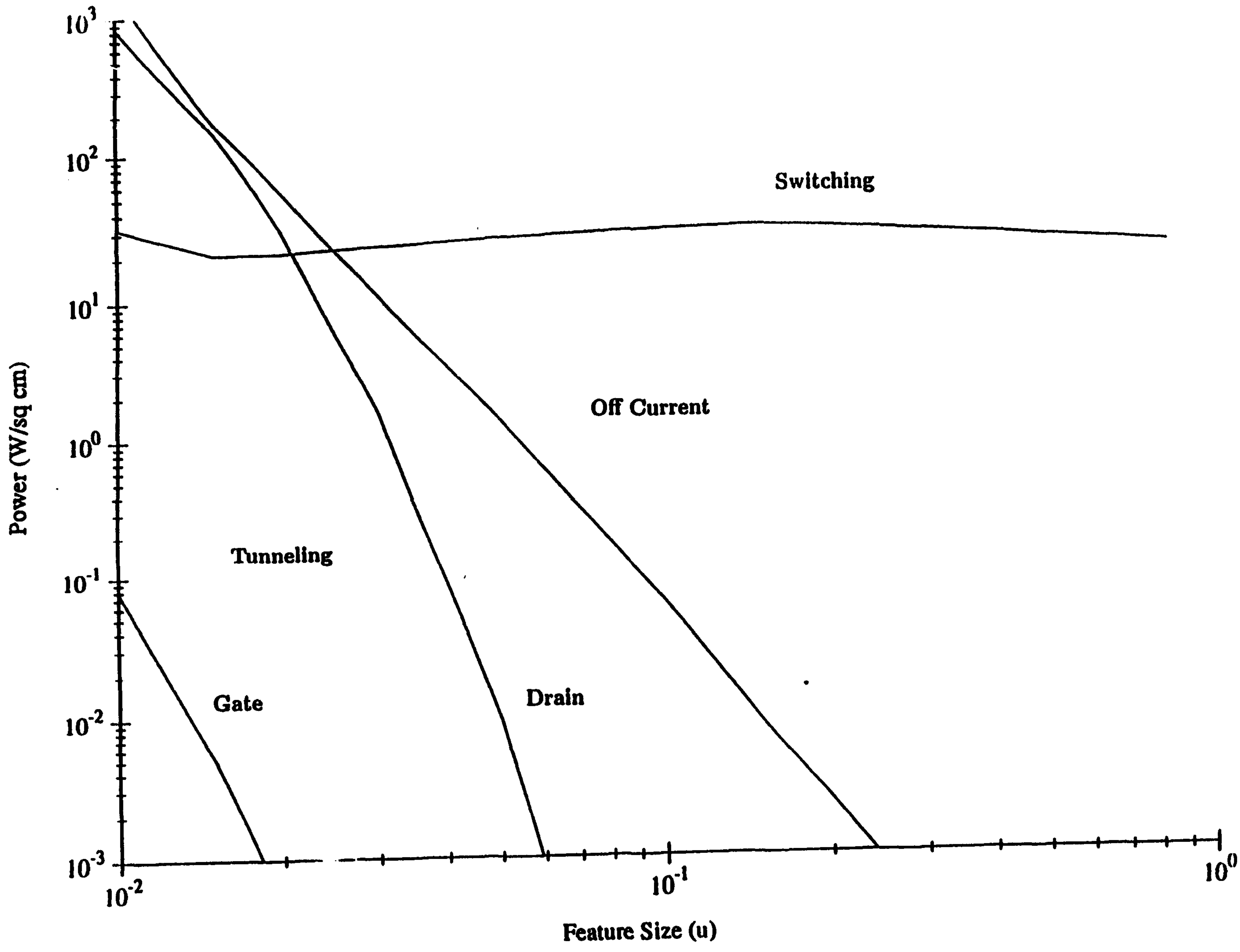
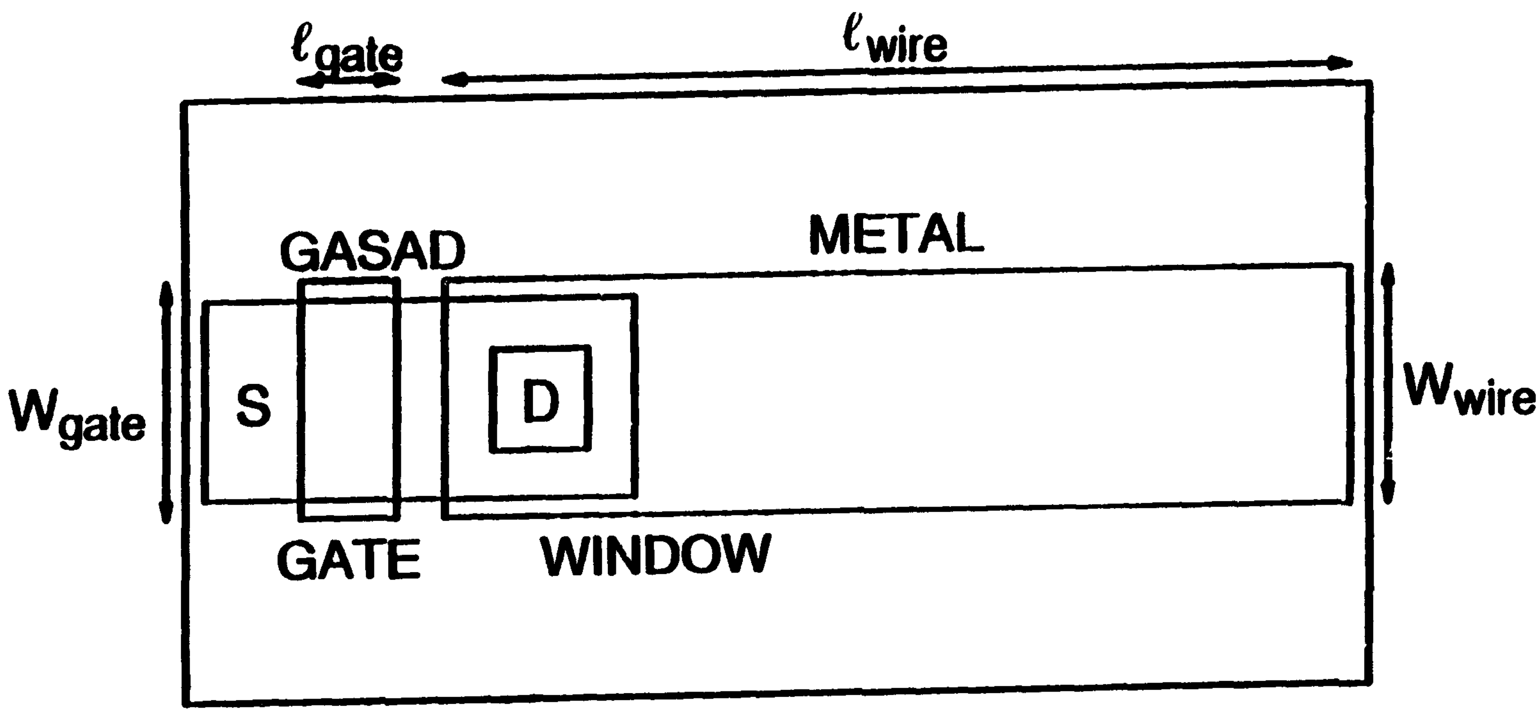

Switching
Off Current
Tunneling
Drain
Gate
Power (W/sq cm)
Feature Size (u)
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-2}
10^{-1}
10^0

DesignRules



- $W_{wire} \approx W_{gate} \approx 2\,\ell_{gate} = 2$ MFS
  - from packing constraints
- ℓ_{wire}
  - depends on time to charge parasitic capacitance

AT&T Bell Laboratories

Apr 18 19:10 /intrigue.3g/colin/metal/design.rule

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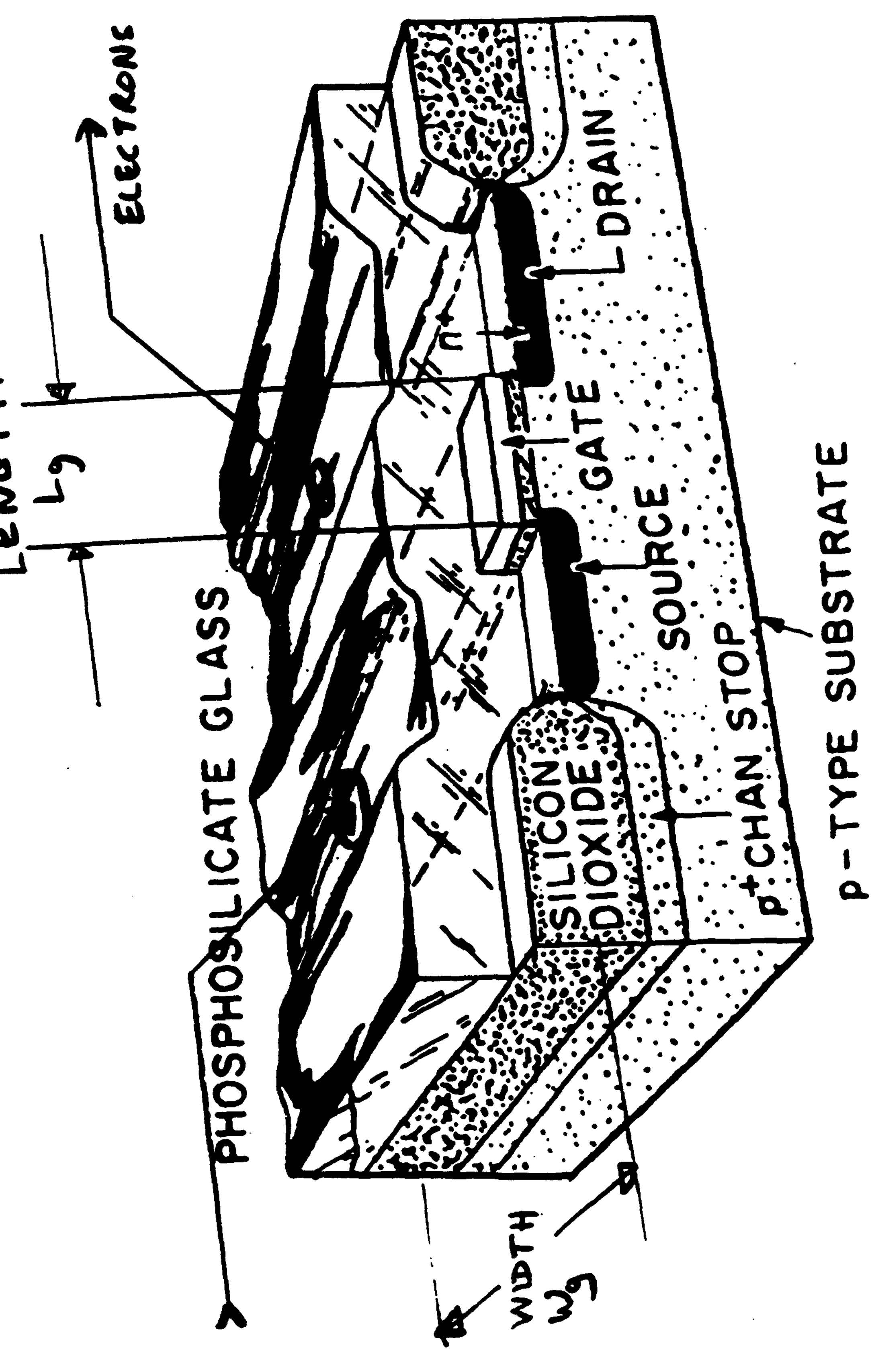
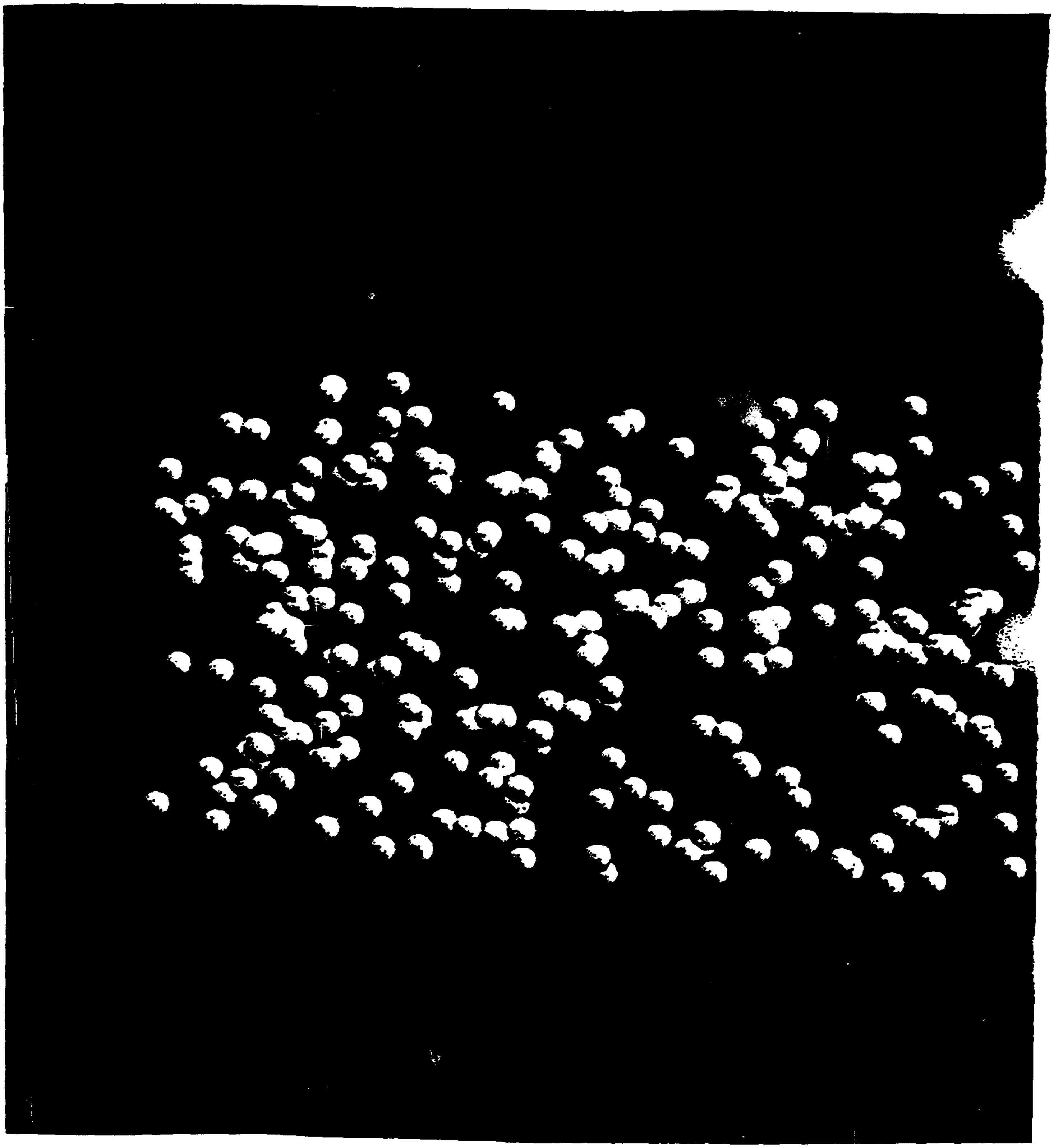
Consider a "typical" ultrasmall device, with gate of 50×100 nm:

- For inversion density of $2 \times 10^{12}\ cm^{-2}$, there are only 100 electrons in channel under the gate when the device is fully in the on state.
- Charging and discharging of single impurities can lead to fluctuations of 40-50% of total conductance if quantum effects become important.
- Total conductance of device is only 4-6 times the quantum unit of conductance.
- Expected variations in surface smoothness of oxide-semiconductor interface are 20-40% of nominal oxide thickness.
- Contacts are expected to be quite granular, leading to "hot" spots in current injection into channel, further exacerbating any quantum effects.



ELECTRONS
LENGTH
L_g
DRAIN
n
GATE
SOURCE
PHOSPHOSILICATE GLASS
SILICON DIOXIDE
p^+ CHAN STOP
p – TYPE SUBSTRATE
WIDTH
W_g

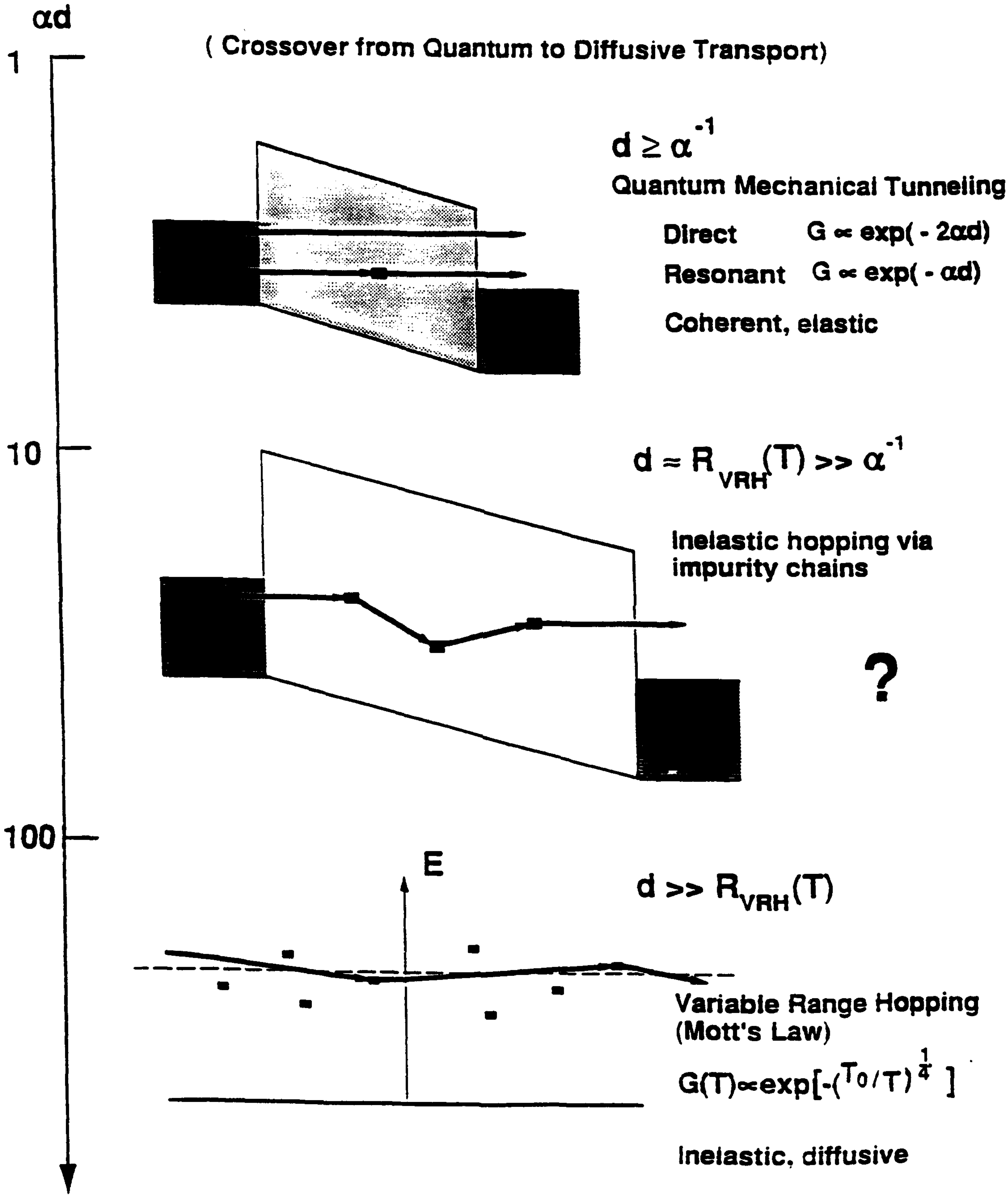


Random atoms

- Alloys
  - Energy gaps
- Heavy metals
  - Recombination centers
- Donors, acceptors
  - Band tails/Impurity bands
  - Energy gap
  - Random electric fields
    - impurity spectra
    - impurity conduction
  - Conductivity fluctuations

Tunneling Via Localized States

(Crossover from Quantum to Diffusive Transport)



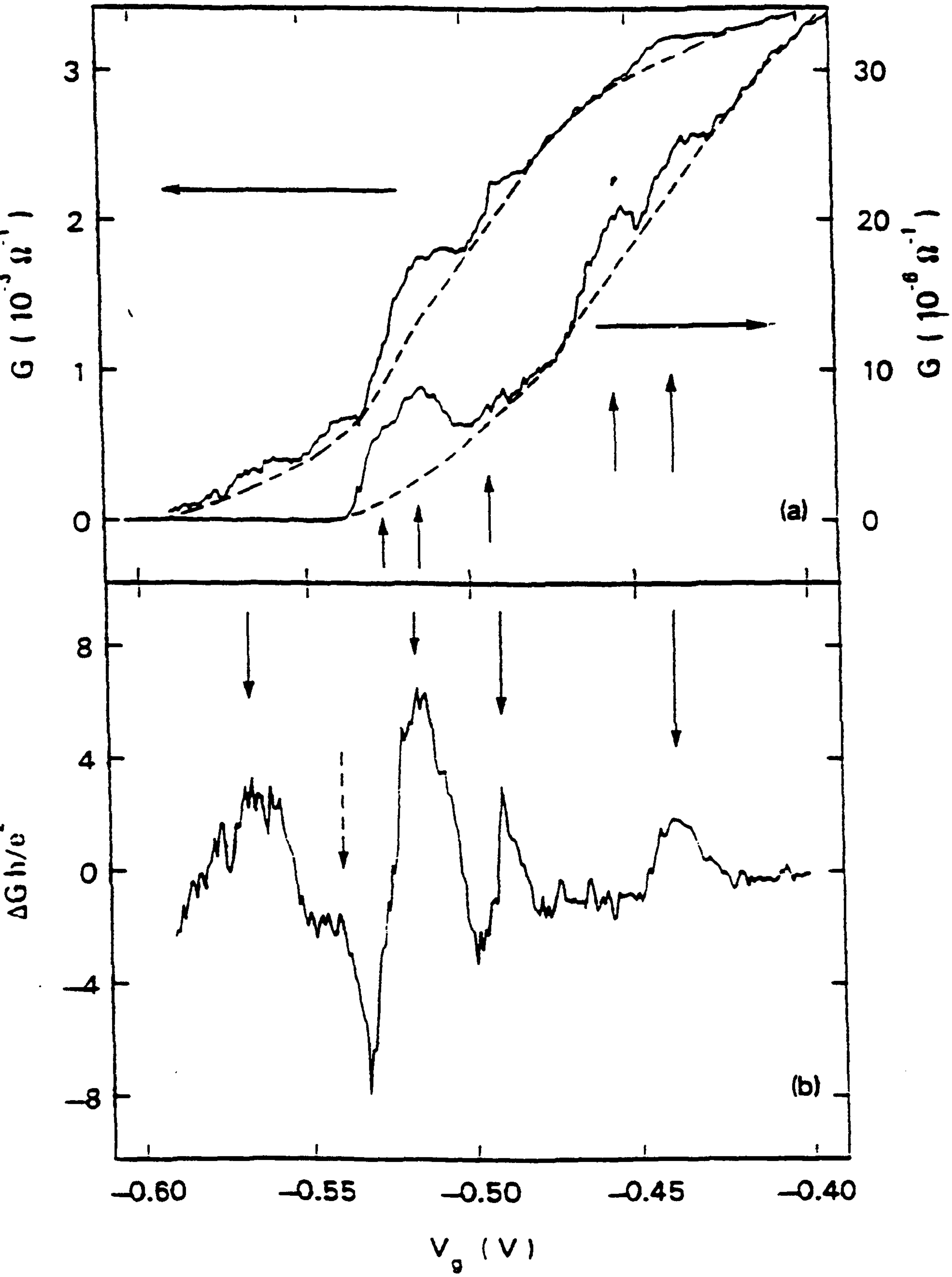


FIG. 2. The dependence of the conductance $G(V_g)$ on gate

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Recommendations to ARPA:

- A large-scale program for study of fluctuations is *not* warranted; effects are expected to be sample specific.
- An expansion of ULTRA program to allow studies of the impact of fluctuations in devices studied under that program would leverage both the ULTRA program and its impact on future ULSI.
- Studies of conventional scaling below 100 nm should also include considerations of statistical fluctuations.

STATISTICAL LIMITS OF ULTRA-SMALL DEVICES

Workshop Coordinator: David K. Ferry

July 12, 1993

8:00 am	General Introduction, Dave Ferry (DSRC/ASU) and Jane Alexander (ARPA)
8:15 am	"Scaling, Randomness, and Limits in Semiconductor Devices," Bob Keyes (IBM)
9:00 am	"Limits on Gigascale Integrated Circuits: When Will the Bubble Burst?", Colin Warwick (ATT)
9:45 am	Break
10:00 am	"Fluctuation Phenomena in Lithography and High Density," Fabian Pease (Stanford University)
10:45 am	"Real-Time Process Control of Growth: Problems," Dave Aspnes (NCSU)
11:30 am	Discussion
12 Noon	Lunch
1:30 pm	"Fluctuations in Film Growth," Stan Williams (UCLA)
2:15 pm	"Quantum Fluctuations in Ultrasmall Devices," David Ferry (DSRC/ASU)
3:00 pm	Discussion

STATISTICAL LIMITS OF ULTRA-SMALL DEVICES

Workshop Coordinator: David K. Ferry

July 13, 1993

8:00 am	"Impurity Fluctuations and Contacts", Tom McGill (DSRC/Caltech)
8:45 am	"Statistical Effects in Thin Film Leakage", Mac Beasley (DSRC/Stanford University)
9:30 am	Break
9:45 am	"Fluctuations and Systems: Universal Aspects or Only Messy Details," Rolf Landauer (IBM)
10:30 am	"How Small Can Devices be Made to Work in Circuits", Carver Mead (DSRC/Caltech)
11:15 am	Wrap-up Discussion
12:00 Noon	Lunch

STATISTICAL LIMITS OF ULTRA-SMALL DEVICES (DAY 1)

July 12, 1993

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STATISTICAL LIMITS OF ULTRA-SMALL DEVICES (DAY 2)

July 13, 1993

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EHRENREICH, Henry	DSRC/Harvard	617-495-3213
EVANS, Drew	DSRC/CE&A	415-369-4567
FERRY, D.	DSRC/ASU	602-965-2570
GILBERT, B.	DSRC/Mayo	507-284-4056
HENDRICKSON, Brian	USAF/RL	315-330-7667
HESS, Verne	NSF/DMR	202-357-9789
HEUER, Arthur	DSRC/CWRU	216-368-3868
HU, Evelyn	DSRC/UCSB	805-893-2368
HUSAIN, Anis	ARPA/WPI	703-693-2236
JUNKER, Bobby	ONR	703-696-4212
KAILATH, T.	Stanford Univ.	415-723-4628
KEYES, R. W.	IBM	914-945-2040
LANDAUER, Rolf	IBM	914-945-2811
LARRABEE, Graydon	DSRC	214/239-0008
LEHENY, Bob	Bellcore	908-758-3203
LEMNIOS, Zachary	ARPA/MTO	703-696-2278
LYTIKAINEN, Bob	DSRC/ARPA	703-696-2242
McGILL, T.	DSRC/CalTech	818-356-4849
MEAD, Carver	DSRC/CalTech	818/395-2814
MURPHY, James	ARPA/ESTO	703-696-2250
OSGOOD, Richard	Columbia Univ.	212-854-4462
PATTERSON, David O.	ARPA/MTO	703-696-2276
PEASE, Fabian	Stanford Univ.	415-723-0959

RAPP, Robert	DSRC/Ohio State Univ.	614-292-6178
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SINNOTT, M. J.	Univ. of Michigan	313-764-4314
SROLOVITZ, David	DSRC/Univ. of Michigan	313-936-1740
TING, David	CalTech	818-395-4779
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ADVANCED LITHOGRAPHY

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EXECUTIVE SUMMARY

Objective of Workshop

The state of advanced lithography has advanced to the point where there are a significant number of options, and considerable dispute over the selection of a "lithography of choice" for future generations of integrated circuits. In this workshop, it was hoped that a candid, thorough discussion of the current situation of lithography for the semiconductor industry could be obtained. Representatives from all major lithography programs (currently thought to be viable) were present and each speaker was charged with:

Providing an overall view of the particular technical approach being represented and the way the advanced lithography function is accomplished.

Providing a complete description of the lithographic process for the particular method, including original pattern generation, pattern transfer, pattern development or mask, resist, and exposure, where required for the method.

Indicating the relative strengths and weaknesses of the method, in comparison to the others, for each ingredient of the lithographic process.

Providing a road map with indicated areas where effort is required to provide successful lithography at 0.18 µm, 0.12 µm and below.

Additional information was gathered in our month-long study of this project. The results in this report integrate the outcome of the workshop discussions with a number of industrial lithographers and a technical assessment of the literature.

DoD Relevance

Lithography is the key to making modern electronic chips. It sets the density of devices by determining the minimum feature size and the degree to

which we can align the multiple mask steps that characterize a modern semiconductor process. The military importance of the highest performance, high density electronic systems is of little dispute. Hence, the ability of the US to control the production of high performance electronic chips for military applications is a major defense objective. Further, large-scale integration in electronic chips is one of the best examples of a dual use technology. In fact, the drive to denser integrated circuits, which have been a mainstay of the civilian computer and electronics industry, was originally led by the need for reliable, robust electronics for missile applications. In this regard, advanced lithography is the enabling technology for the $300B electronics industry.

Scientific and Technological Summary

The scientific and technical issues in future generations of advanced lithography are contained in the attached detailed text. In brief, however, one of the central conclusions of the meeting is that lithography based on exposure with optical wavelengths longer than 150 nm will be the dominant lithography tool through the early years of the next decade; e.g., optical lithography, using excimer lasers and phase-shift masks, will be the tool of choice for almost all lithographic tasks for the next several generations of ULSI chips. This is expected to be the case until integration requires design rules (and finest line control) below 0.18 μm, the latter of which will be required for the 1 Gb DRAM by 2001. While the next generations (0.12 and 0.1 μm) may well be optical as well, it is expected that a transition may begin to other techniques, such as: proximity x-ray, projection x-ray, direct-write e-beam, projection e-beam, and projection ion-beam. To have a significant impact in this time frame, product readiness will be required by the year 2004, and demonstration of alignment and exposure capability will be required some 2-3 years earlier. The transition may begin earlier, as the high cost of phase-shift masks may preclude their use in low volume random logic chips.

Conclusions

The current situation in US industry, in which a commercial vendor of lithography production tools is almost non-existent (those currently surviving are in severe financial difficulty), has led to a number of government-sponsored programs designed to give the US an indigenous industry in this area. While these programs have been well intentioned, they have not produced the desired

effect. Although they were carried out with a manufacturing customer (Intel, TI, Motorola, IBM, AMD...) providing both input and some commitment to purchase the developed product, the number of machines actually purchased has been limited. An example is Sematech's attempt to save the GCA effort, in which initial efforts to develop an excimer-laser stepper were converted into the development of an I-line (365 nm) stepper, and resulted in a product that was over a year behind schedule for the industry purchasing decisions and lacked the optical stability (the lens had to be designed, but the new Tropel lens is thought to be very good) and ease-of-use of the Japanese competition.

The current trends and tendency to evolution rather than revolution in this very-high capital cost industry is likely to make optical lithography the production tool of choice for generations requiring resolution at and below 0.25 μm. It is possible that it might even be extended (e.g., using Fourier techniques) to 0.1 μm. However, below 0.1 μm, non-optical methods are likely to be employed. These latter lithographic tools will not be required before 2007. Hence, adequate research and advanced development can be accomplished over the next fifteen years. Techniques, such as proximity X-ray, which have been brought to a very high level of technical readiness, but appear to lack a production role, provide a painful illustration of the toll in economic and human resources that such premature rushes to technical development can lead.

A major effort in optical lithography should allow us to be assured of having the option of producing our own exposure tools should the foreign companies decide to limit our access (a point of some concern to many in the industry). GCA and SVGL with their deep UV capability, and the current level of interest by the production industry in this country, could provide a solution for our next generations of manufacturing needs. Major efforts in mask, resists, and Fourier optics could give us a competitive advantage even while employing the foreign-supplied exposure systems. Research and development in non-optical techniques can also develop cost effective processes for use in the cluster-tool environment envisioned for ARPA's future fabs for small numbers of high performance chips. However, to be consistent with the cluster-tool philosophy, the tool should be small and modular.

Development of advanced lithography methods for sub-0.1 μm could allow the US to gain a competitive advantage in exposure tools at the point for which the change from optical lithography/technology occurs. On the other hand, it should be noted, the competition (e.g., the Japanese) are pursuing a

multitude of projects on each of the major possibilities for lithography of choice. Nevertheless, an intelligent program of research and development can provide needed components for retaining a U. S. provider of lithography tools. Despite the long lead time for these advanced techniques, proper timing and attention to the equipment requirements of the customers is still required during the development period. Failure to adequately address the timing and customer acceptance issue could result in programs with the difficulties of the current proximity X-ray lithography program.

Suggestions for actions by ARPA

We propose two sets of ARPA actions: those involving near-term programs, and those involving long-term programs.

Near-Term

We recommend that ARPA avoid near-term lithography objectives. Industry, particularly SEMATECH despite its record with GCA, can best describe market-driven programs that can result in products acceptable to, and "bought into" by, the American semiconductor industry. In this category, we include the current efforts at GCA and SVGL as well as the proximity x-ray lithography program with its current very high level of readiness.

Long-Term

Long-term programs are more consistent with the successful ARPA style of generating a tech base that may later be commercialized. We suggest that ARPA consider:

A basic program to extend the fundamental limits of optical lithography. The effort should include development of resists, masks, and Fourier optics, especially those compatible with cluster tools and control of the process. Notably, the effort should investigate advanced Fourier optical techniques to produce advanced (cost effective) phase-shift masks, and design tools for these masks that might make them more appropriate for random logic chips. Resists that are appropriate for the shorter wavelength sources, and can be used with the advanced optical techniques, should be sought.

The proximity x-ray program has successfully developed a tool that has proven to be useful at 0.25-0.35 μm, but is not likely to supplant optical techniques at these design rules. Questions about the stability of overlay, mask

technology, and the manufacturability due to very small proximity gaps at resolutions of 0.1 mm and below should be addressed, if this is to be a candidate for future lithography usage. Further, efforts should be made to develop point sources that will alleviate the problem of granularity inherent in the current synchrotron-based approach. The possibility of usage in the intermediate resolution range is best left to SEMATECH, as the questions are of manufacturing compatibility and cost effectiveness in replacing the optical incumbent. They are not ones of research and development. It seems that the question is whether or not proximity X-ray can reach the smaller resolutions expected in the future.

The projection X-ray program should be focused on demonstrating feasibility of the approach. The reflection mask technology and multi-layer metallic film optics should be the subject of small research efforts. Resists appropriate to the longer wavelengths used in this approach should be sought. The effort should be coupled more closely to industry with the hope of avoiding the development of a non-production-ready product. The effort should be kept small, appropriate to a long-range research program, until the basic underpinnings are in place.

The projection e-beam approaches being pursued at AT&T Bell Laboratories (SCAPEL) and IBM Research (PREVAIL) should be tested for their feasibility, with an eye to testing the overall throughput achievable and to be assured that charging effects do not reduce the level of resolution and overlay attainable over the entire field beyond acceptable limits. Attempts to produce a multiple-beam source are interesting and should be continued at the current research level until feasibility and stability is demonstrated.

The projection ion-beam approach at MIT/IMS should be tested for feasibility. Because of the short range of the ions, stencil masks required in this technology should be investigated thoroughly to test their feasibility. Special resists, which can used in thin layers (or in thick layers where the ions stop in the resist) should be investigated for this application. The questions of resolution, overlay precision, intra-beam ion repulsion are crucial (and controversial) and should be investigated.

While currently severely limited by throughput, the scanning tunneling microscope could be the ultimate in resolution and overlay for electron-beam lithography. Small research efforts should be continued to develop the lithographic process. Efforts to improve the throughput by various technologies, including using multiple tips, should be investigated.

BACKGROUND INFORMATION ON ADVANCED LITHOGRAPHY

T. C. McGill, D. K. Ferry, E. Hu, and R. H. Osgood

1. Introduction

Lithography is the key to all of the planar integrated circuits built today. The lithographic process is used to print (in the Si media) the patterns of doping, insulators, and metals that make up the functional integrated circuit. This position is likely to continue for the foreseeable future. This process defines the fundamental scale of the devices and represents roughly 1/4-1/3 of the cost of producing a chip. Today, each lithographic "exposure" is achieved by exposing a small area at one time, termed the field-of-view (currently approximately 20 x 20 mm), and stepping from one area to the next until the entire wafer is exposed. The machine that does this is called a stepper, and Nikon and Canon dominate the market. One other major player is AMS Lithography, a Dutch company. It should be pointed out that these machines are reduction technologies (such as 4-5X), where a 0.5 μm feature on the chip requires only a 2.0 or 2.5 μm feature on the mask.

The US history in lithography tools is very troubling. Originally the US dominated the commercial stepper business. Both GCA and Perkin-Elmer (the lithography effort is now part of SVGL) had major market shares during the recent past. However, the US companies allowed themselves to become vulnerable (it is often suggested that these companies lost sight of their customer needs) to Japanese competition and the willingness of Japanese companies to buy the market with what are thought to be very small or negative margins on their equipment.

This loss of dominance is perceived as a major national threat, because of the importance of lithography to a major industrial segment of the U. S. economy. The overall perceived threat has been used to argue for heavy government intervention, one result of which is SEMATECH, and more specifically, the lithography threat led to the Congressionally-mandated X-ray lithography program. While the government intervention has been well-intentioned,

the results have been less than spectacular in improving the US position in providing lithographic exposure tools even for our home industry. As with many programs of this type that are generated by technological dreams and not by market realities, there has been a failure (by all parties) to recognize the advantage of an incumbent technology, optical lithography, and its ability to adapt and improve its performance based on the learning curve. This is complicated by the fact that it costs a considerable amount (some estimates are $100-200M to produce and market a stepper even after development work is complete).

2. History of the Current ARPA/SEMATECH Involvement

The government efforts in lithography have been substantial programs with a generally good record of technical achievements that, however, were started largely through the government processes and not always as a result of market pull, as industry leaders continued to look ahead with sometimes divergent views. Hence, these programs are perceived (perhaps wrongly) to have failed to produce products that have industry buy-in, or even successful products in a market sense.

2.1 GCA/SEMATECH

Originally, as mentioned above, GCA was a major supplier of lithography tools. However, it is perceived that GCA lost touch with the needs of its customer base. Consequently, GCA's market position became vulnerable, and as new generations of steppers appeared, they lost significant market share.

In contrast, Japanese manufacturers took an aggressive position to achieve a significant share of the market, but often with products that contained copies of significant parts of U.S. products. Nikon is thought to have offered aligners on a "guaranteed basis," e.g., use their lithography tool in production and Nikon would cover the cost of any lost production time and/or profit. Nikon, in fact, may have incurred a substantial loss to enter the market. Nikon made major efforts to satisfy customer needs, and their current stepper is felt to be extremely user-friendly. A similar story of commitment to the customer surrounds the entry of Canon into the market, and they also are considered to have a very user-friendly stepper. These two companies, along with ASM Lithography, currently dominate the market in steppers.

As their market share declined, GCA became somewhat concerned. A major restructuring of the company, with new management, occured in 1987.

GCA sought to initiate a government-sponsored program in the late 1980's to seek a technical leap over the Japanese competition through the development of an advanced stepper using an excimer laser source (a technology that is expected to be needed for the 256 Mb DRAM in 1998, but applicable to earlier generations of chips). A cooperative program through Sematech was initiated in 1989. Then, it was realized that the market did not demand the very-short-wavelength, excimer-laser-based stepper (initially it was not thought that the I-line would be able to be used at 0.5 mm) soon enough for GCA to survive financially through to its introduction. Hence, there was a dramatic reversal in approach which led to GCA concentrating on an I-line stepper for the near-term market. It is thought that GCA received approximately $54M in Sematech support. With this support, GCA reached the market-place with their I-line stepper, but did so roughly one year too late. That is, the major acquisition decisions for this product had long-since taken place, with the market being captured by Nikon and Canon. Several factors are thought to also hurt the introduction of the GCA's product: 1) it is not thought to be as optically stable (there was a necessary lens redesign by Tropel for GCA) as that of Nikon and Canon products, and 2) there is residual antipathy toward GCA in the industry, presumably as a result of some perceived lack of concern for their customer needs earlier in their history. Hence, GCA has not achieved adequate market penetration with their I-line stepper, and is again in severe financial difficulty.

2.2 Proximity X-Ray Program

A similar pattern emerged with the proximity x-ray program and has resulted in much the same outcome. Congress mandated a program in X-ray lithography, presumably to support the Congressionally-perceived needs of constituents at universities in Louisiana and Wisconsin. While it was originally planned for the program to be assigned to DoE, it ended up with DARPA because of the latter's widely-perceived experience in making connections with the important components of the semiconductor industry. Under DARPA's direction, NRL, IBM, ATT, and MIT joined the effort, which resulted in the addition of experience (and, some say, credibility) to the program. This Congressionally-mandated program has involved very substantial equipment purchases, and the program was funded at a level of approximately $70M/year. And, this estimate does not include the even larger amounts of internal IBM funding that went into the program and facility. IBM, NRL, MIT, Wisconsin, in their combined effort, succeeded in producing a viable technology for

0.35 μm and reached a high degree of technical readiness. IBM even constructed a superconducting synchrotron for $30M, and demonstrated that X-ray gives a smaller critical width to the production of critical dimensions, which could produce a better product. IBM has demonstrated a 512Kb SRAM, but with overall yields which are quite low. The IBM program was initially targeted at 1.0 mm, then 0.5 μm, and now 0.35 μm, as optical stepper technology has progressed and continued to dominate the applications. The industry, however, has already committed to the use of the easier optical stepper technology at this latter dimension, so that there is little market share available to the expensive synchrotron-based technology. Moreover, the technology is a proximity technology, in which the thin membrane masks are 1X and the mask is held in very close proximity to the wafer. IBM has attempted to form a consortium to maintain and continue the proximity X-ray effort. Given the industry's reluctance to commit to their own synchrotrons, it seems unlikely that the IBM consortium effort, even if it should be initiated, will result in a product used by U.S. semiconductor manufacturers.

3. Terminology

3.1 Lithographic Process

The lithographic process consists of the creation of a pattern in a material that is later processed to transfer the pattern to the material. Most patterns are transferred from a mask to a resist material that is specially tailored to be exposed by photons or particles passed by the masking filter. There are three different mask wafer configurations: a contact one in which the wafer/resist is in hard contact with the mask; a proximity one in which the wafer/resist is near the mask; and a projection one in which the image is projected by a lens system onto the resist/wafer combination. The industry has progressed from contact to projection lithography over the past few decades. One method that does not involve the use of masks is the so-called direct-write e-beam in which the electron beam is rastered over the field writing individual pixels, or a few hundred pixels in the case of a shaped beam with a mask. While the use of direct write e-beam makes it difficult to produce the throughput necessary for full-scale wafer production, it is the best method for generating high-resolution masks.Hence, the lithographic process in general requires: masks, resist, and an exposure tool. Each of these must meet certain criteria for a fully successful lithographic process.

3.1.1 Masks

The Mask has to be able to pass the beam in the areas that are to be illuminated and to stop the beam in the areas where we want no exposure. With the need for higher-resolution beams, we are being forced into shorter wavelength sources: deep UV photons, e-beams, x-rays and high energy ions. The flux of energy from the source is quite high resulting in substantial energy deposition in the mask. Masks formation, durability, inspection and repair must all be within the tolerances and economic constraints set by a manufacturing environment. Note that the mask technologies for optical, X-ray, e-beam, and ion-beam lithographies are based upon very different mask-substrate structures.

3.1.2 Resist

The resist (photographic emulsion for the lithography process) is material which alters its chemistry upon exposure and which allows the transfer of the image carried by the beam. Some critical parameters are: stability, sensitivity, ease of development, uniformity of deposition, non-linear response during the exposure process to enhance the contrast. Overall the simplicity of use must be such that exposure process and development leads to successful transfer of the process. Most of the resist materials are organic. The exposure process either makes the material less soluble (usually by cross-linking a short-chain polymer) in the chosen developer in the area of exposure (negative resist) or makes it more soluble (by scission of long-chain polymeric material in a positive resist).

3.1.3 Exposure Tool

There are three different basic approaches to exposure with a mask—contact printing, proximity printing and projection printing.

Contact printing is the simplest and is in principle capable of very high resolution because it minimizes optical diffraction. In this technique the mask is brought into intimate contact with the substrate/resist and then the exposure is made. While this method of printing gives high resolution, it is now not viewed as being manufacturable since the resist frequently sticks to the mask, which in turn ruins the mask and creates defects in the wafer. Further, the process of bringing the mask into intimate contact with the resist/wafer can break the wafer.

The proximity process is one in which there is a small gap between the masks and the resist/wafer combination. In this case the resolution is limited by the near field aspects of the problem. It is given by

$$W = K\sqrt{G\lambda}$$

where K is a constant roughly (0.83 for proximity X-Ray), G is the gap and l is the wavelength of the exposing radiation.

Projection lithography uses a lens system to project the image produced by an illuminated mask onto the resist/wafer. The resolution of the projection optical system is limited by the diffraction effects of the lens system. The resolution W is given by

$$W = K_1 \frac{\lambda}{NA'}$$

where K1 is a constant which is classically equal to 0.5 but which can take on other values related to the process, l is the wavelength, and NA is the numerical aperture. The depth of focus d is given by

$$d = K_2 \frac{\lambda}{(NA)'^2}$$

where K2 is a constant. Combining the two equations, we have that

$$d = \frac{K_2 W^2}{K_1^2 \lambda}$$

Hence, we have that for fixed resolution the depth of focus increases with decreasing wavelength. Depth of focus should be as great as possible both to provide for errors in focusing but also to make it possible to work with the nonplanar structures within the focal area on the wafer. We also point out that a popular approach is reduction projection step and repeat techniques which have the advantage of relaxing some tolerances on mask fabrication and defects (e.g., 5X reduction for 0.25 mm means minimum feature on the mask is 1.25 mm; also some defects on mask won't print when reduction is used).

The exposure tool must carry out a number of functions with accuracy, reliability and speed. For stepper systems, the exposure tool must position the wafer and then bring the local region into close alignment to allow for overlaying a number of masks steps with high resolution. The stepper typically adjusts each local region before exposure to improve overlay. In recent years, automatic leveling of the local region on the wafer has been introduced to compensate for the lack of optical flatness of the wafer. The alignment and exposure processes must be carried out with sufficient speed to make the economic processing of wafers possible. Typically, current processes require many 10's of masking steps. Hence, the number of pixels that must be written per sec (Rpixel)is given by

$$d = N\left(\frac{d_w}{W}\right)^2$$

where N is the number of wafers per unit time that must be written, dw is the diameter of the wafer, and W is the resolution. Typically in today's fab with 5000 wafer starts per week, say 20 mask steps, and 50 wafers/hour for a single aligner, the number of mask aligners would be 12 if we had 100% utilization. Since aligners are multi-million dollar pieces of equipment, cost of the aligners alone can be a significant item in the overall capital equipment for a fab.

The current tendency in the industry is to go to larger wafers, smaller resolutions, and larger number of masks steps. All of these tendencies push for increasing the writing rate. It is these demands that have precluded the use of the direct e-beam or ion writing techniques. Basically the mask techniques allow us to write lots of pixels in parallel.

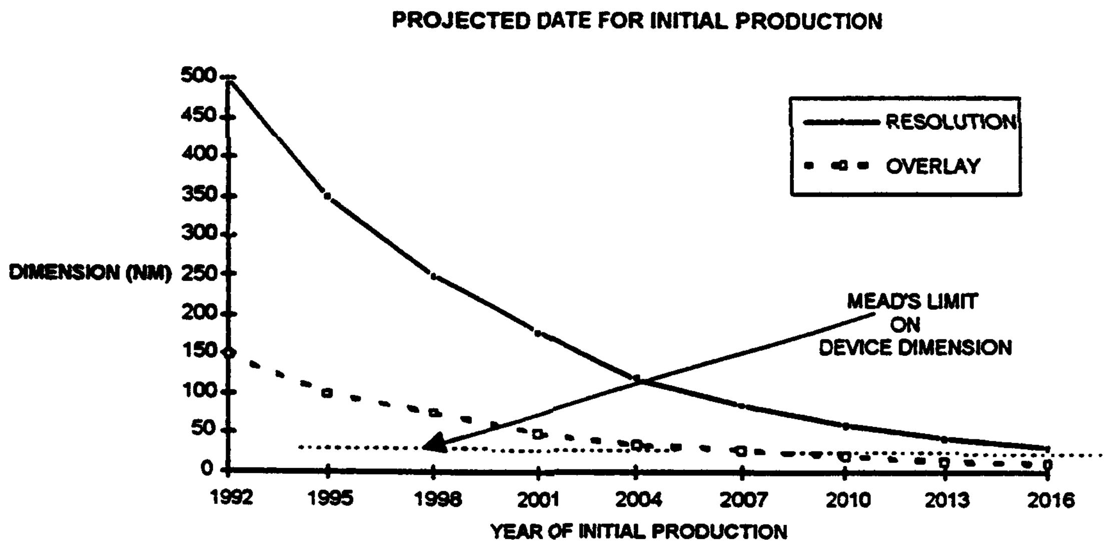


Figure 1. The projected resolution and overlay dimensions as a function of initial year of substantial production. The limit indicated by C. A. Mead is also indicated. Projections for years after 2004 are based on a doubling of the density every three years.

3.2 Time scale for evolution of semiconductor industry

The major consideration for lithography is the evolution of demands for resolution with time. In Fig. 1, we have taken the numbers from the SIA roadmap for resolution and overlay. We have extrapolated these numbers for the period beyond 2004 to what is believed to be the ultimate limit on the

MOSFET technology of 0.03 mm devices. This plot assumes that the rate of size reduction will continue with roughly a doubling rate of density every three years. Moore of Intel has been questioning this rate given the very high capital costs that are beginning to be encountered in these fabs and the projected rapid increase in fab cost with decreasing feature size. Hence, estimates for when a given resolution in lithography will be required are likely to be early if they are based on these curves. The date for pre-production testing of a lithography tool at the present is roughly three years before the start of production. We will assume for our projections the current time schedule for evolution continues as the time at which most research and development must be completed.

Source	Wavelength (nm)	Resolution Lower Limit (nm)	Depth of Focus (nm)	Minimum Reported Dimension	Projected Minimum Dimension with Phase Shift Masks
g-line in Hg Source	436	311	668		299
i-line in Hg Source	365	261	558	250[6]	250
KrF Excimer Laser	249	178	381		171
ArF Excimer Laser	193	138	296		132
F_2 Laser	157	112	120		108
Projection X-ray	13	33	244	40	N/A

***Table I.** The available optical sources and the lower limit on resolution using K1=0.5, K2=0.75, and NA=0.7 (except for X-ray, where the NA=0.2). For comparison in the case of I-line we have indicated a result from an experimental 64Mb DRAM fabricated using phase-shift masks at Hitachi. Assuming this scaling would hold at all dimensions, we have used this to project an ultimate limit using phase-shift masks in the last column.*

4. Current Technical Status

We will attempt to highlight some of the technical issues we have found by discussing the technical status of each of the techniques.

4.1 Projection Optical Steppers

Optical steppers are the current incumbent technology.

4.1.1 Masks

Masks are formed by metallic layers on fused quartz substrates. The masks are prepared by direct-write e-beam to attain the resolution. The current masks are fairly simple but efforts are now under way to utilize phase-shift masks. These masks will contain pattern phase shifting layers that will use the interference between the partially coherent waves to partially cancel the diffraction phenomenon and, hence, produce higher resolution and greater depths of focus.

4.1.2 Sources

There are a wide range of optical sources available ranging from the currently employed lines from a high-intensity Hg lamp, to various excimer lasers. A list of the sources, with their wavelength, and optimistic estimates of resolution is contained in the table below.

4.1.3 Resist

Currently, resists are available for i-line. The current deep UV resists ($\lambda<249$) are rather difficult to work with. The IBM/APEX resist has a very limited process window, measured in minutes. However, new resists are in development at a number of the classic sources of resist.

While optical techniques can be projected to reach below 0.12 mm with the F2 excimer laser, it should be noted that this begins to require a high vacuum environment, which will dramatically increase stepper cost and lower throughput. We envision that this will be the point at which changes away from optical lithography will begin in earnest.

4.2 E-Beam Direct Write

Direct-write e-beam has been available for a number of years. Single e-beam tools have been used to write "mask" levels directly on the wafer for speciality circuits at IBM and have been used to produce masks. However, it widely felt that the throughput for a single-source direct write is too slow to be used in a production facility.

4.3 Proximity X-ray

Proximity X-ray has also been around for a long time. It does not suffer from the throughput limitations that have constrained direct-write e-beam. For a number of years, it has been viewed as the replacement for "optical lithography" when it arrives at its ultimate limit. Originally this ultimate limit was viewed as being around 1 mm, but this proved not to be the case, and proximity X-ray has been pushed down to try to keep up with the progress in optical steppers. However, it suffers from the limitation of any proximity method; that is, the need for a small gap to obtain high resolution. Using a wavelength of 1nm and a gap size 12 mm in the equation above one obtains an ultimate resolution W=100nm. While much smaller gaps could result in smaller resolution, the manufacturability of lithography with such small gaps between resist/wafer and masks is in doubt.

The efforts at IBM, NRL, ATT, MIT, the University of Wisconsin, and Louisana State University have brought proximity X-ray to a high level of technical readiness. It has been used to fabricate interesting chips at the 1mm, 0.50 mm, and 0.35 mm limit. Unfortuately for X-ray proponents (but not unfortunately for industry), at each of these levels the necessary optical resolution has not been reached in spite of earlier predictions about such a limit.

4.3.1 Masks

The masks consist of heavy metal absorbing regions patterned on a thin membrane. The membrane is supported on a more extensive structural support. Mask deformations during use are still considered to be a concern in a production environment.

4.3.2 Sources

This technique requires hard X-rays of approximately 1 nm. To obtain a sufficiently intense source, two methods have been pursued: 1) a synchrotron source, and 2) a laser-plasma source. A synchrotron produces radiation by the acceleration of electrons around a closed orbit. The cost of such a source is typically a few tens of millions of dollars. A single synchrotron source could support a number (10-15) of beam lines to harvest the X-rays produced around the entire ring. The laser plasma source heats a very small amount of material to produce a very hot plasma which has a blackbody radiation peak at the desired short wavelength. This source, which has very different spectral and optical properties than the synchrotron, would in principle be preferable to the synchrotron source which suffers from very high initial cost commitment and

lack of granularity for ramping up production.

4.3.3 Resist

We are unaware of any particular difficulties with resist technologies. In fact, the coherence of the X-ray synchrotron sources has enabled the production of high aspect ratio features in single-layer resist, something which is generally achievable in optical and e-beam resists only through multi-layer resist schemes.

4.4 Proximity E-Beam

Proximity e-beam tries to make up for the slowness of direct-write e-beam by using a larger, shaped beam and a mask to generate portions of the pattern. The portions of the pattern may be viewed as characters which would be written all at one time.

4.4.1 Masks

A membrane or stencil mask is required for this technology. The issues of their ruggedness is still an open question.

4.4.2 Sources

Sources are only now being developed with the appropriate beam parameters.

4.4.3 Resist

We are aware of no special problems with resist for this technology. It has been widely used and e-beam resist technology is fairly well developed.

4.4.4 Exposure Process

Questions still exist about proximity effects in the e-beam exposure process. The high energy electron beam produces a number of back-scattered and secondary electrons that can produce unwanted exposure of the resist. However, the high energy e-beam tends to bury these deeper in the substrate which tends to alleviate the problem.

4.5 Projection E-Beam

Projection e-beam differs from proximity e-beam in that we can have mask dimensions which are larger than the final dimension on the chip. The mask is in front of a final set of e-beam optics. Two major efforts are being pursued in this country, one at IBM (the PREVAIL system) and the other at ATT Bell Labs (the SCAPEL system). Both of these systems are in very early phases of development with prototype equipment to be built over the next couple of years. In this process, one major advantage tends to be the fact that

you avoid tight tolerances on mask placement due to the flexibility in deflecting the beam to desired positions on the substrate.

4.5.1 Masks

A unique mask will be used in these systems, particularly the ATT system. Instead of attempting to absorb the very intense high energy e-beam in a standard membrane mask, the opaque regions of the mask will be obtained by scattering the incident e-beam beyond the acceptance of the projection e-beam optical system. This improved mask design allows much higher voltages to be used in the source. The thin membrane structure is contained in a strutted supporting structure.

4.5.2 Sources

The source for this system is a very high current e-beam. Projected beam characteristics are: 100 kV, about 50 μA of beam current. The projection would be at 4X with a mask wafer separation less than 500 mm and a beam size at the mask of 1 mm. Issues regarding high-current defocusing still need to be clarified.

4.5.3 Resist

We are unaware of any special problems with the resist.

4.5.4 Exposure Process

The exposure process still needs to verified. Notably questions about the control of proximity effects and perhaps radiation damage to underlying device structures from such high energy electron beams require investigation

4.6 Projection Ion Beam

Projection ion-beam is at a fairly early phase. Little has been demonstrated about the efficacy of this approach. However, surface acoustic wave devices have been written at 0.25 mm with 55 keV H2- ions. The technique promises reduced proximity effects because of the very short distance over which the ion deposits its energy. Resolution is very high and depth of focus is also quite high.

4.6.1 Masks

The current proposal is to use stencil masks. Questions of manufacturing with such fragile masks (and the fact that two masks per level are required) are still to be addressed. The stability of such masks in the local heating produced by the high energy ion flux for random logic in particular, and for high throughput in general, is yet to be tested or demonstrated.

4.6.2 Sources

The question of whether sources can be realized with the required properties has yet to be determined. Issues of space charge in the ion optics are still to be resolved. There is also a question as to the size and cost of the equipment for a production tool.

4.6.3 Resist

The very short stopping distance for the ions raises issues about the thickness of the resist layers. Either thin resist layers or multi-layer resists will be required, either of which is still a challange.

4.7 Projection X-Ray

Projection X-ray lithography is being pursued in a joint effort involving ATT and Sandia National Laboratories. Simple estimates based on the formulas for projection optical methods with K1=K2=0.75, λ=13.4nm and NA=0.1 indicates that one might attain a resolution of 0.1mm and a depth of focus of 1 mm, with respectable performance characteristics that could be carried to even smaller resolutions.

4.7.1 Masks

Most work, both here and abroad, is in the use of reflection masks. These proposed masks consist of Ge absorbers on a polymide film and a Mo/Si multilayer reflector that is exposed in the areas where we want the x-rays to be reflected. All of this is placed on top of a substrate. The part that has been demonstrated so far is the pattern absorbing overlayer and mask repair with focused ion beam techniques.

4.7.2 Sources

Two candidates for the source are being considered, a compact synchrotron and a laser-plasma X-ray source. Since the photon wavelength is roughly 10 times that employed for proximity x-ray, the source problem is not as demanding. The requirements are to deliver 1 watt to the masks in a 2.6% bandwidth at 13.4nm. However, unlike the proximity x-ray system projection x-ray requires the production of x-ray optics. The optical system that is envisioned is based on multilayers of Mo/Si to produce relatively high efficency (65%) reflective elements. The practical performance of these mirrors is still somewhat questionable.

4.7.3 Resist

The resist technology for this approach is now being developed as well. The current status is that a tri-level resist scheme using PMMA+Ge has been

demonstrated. Other resists are being developed.

4.8 Scanning Tunneling Microscopy

Scanning tunneling microscopy could be the ultimate direct write technique.

4.8.1 Masks

As with other direct-write techniques, there is no mask.

4.8.2 Sources

Scanning tunneling microscopes with a single tip are inherently too slow. However, multi-tip systems involving large numbers of tips could allow for the "exposure" of large areas in reasonable times.

4.8.3 Resist

Precisely how the lithographic process will be accomplished is unclear. A material other than the substrate may act as the resist. One such material that has been used is CaF2. Other techniques might include direct write into the material making up the devices.

5. Observations

Optical lithography is likely to be the method of choice well into the next decade. The appropriate level of technical readiness for proximity x-ray and direct write e-beam should be maintained in case some unexpected technical show stopper is encountered in the optical path. In establishing the appropriate level of technical readiness for these backup technologies, industry should be asked to play a major role. Consortia involving a major participation by industry would insure that during the period of sustained technical readiness, the efforts will be addressing technical issues that will give it the maximum possible chance to enter the market.

5.1 General

Generally, we feel that ARPA should change the major focus of its program from near term to long range research and development that could smooth the transition when optical lithography has run its course. At the same time we suggest that ARPA assist in providing the US with the maximum tech base to take advantage of optical lithography.

5.2 Specific Challanges

5.2.1 Optical

We need to exploit all of the tech base issues to use the deep UV sources

including the development of phase-shift masks for random logic circuits, and new resist materials for the shorter wavelengths.

5.2.2 Proximity X-ray

The major challenge to proximity x-ray is infrastructure. Who is going to return to proximity printing? Can proximity X-ray be extended into regions where it is not in direct competition with optical and can it seek to have a future in the post-optical era. Some of the issues include: small gaps, mask (1X), overlay and alignment accuracy. The development of point sources would make it possible to solve the inherent difficulties with synchrotrons where large initial investments lead to large numbers of beam lines and very large commitments for economic viability. In essence, the questions with regard to proximity X-ray seem to focus upon whether or not it can be proven useful at the 0.12-0.1 mm range (and below) of resolution.

5.2.3 Direct Write E-Beam

The major challenges to direct-write e-beam are: throughput (cost of ownership), charging effects and total current space charge effects.

5.2.4 Proximity E-Beam

The major challenges are the same as for direct write e-beam with the addition of needing to prove the technical feasibilty of the cell projection technique, although here it is likely to be limited to high volume applications with repeating cells.

5.2.5 Projection E Beam

Some of the issues include the demonstration of manufacturable masks including their repair, the role of the proximity effect, space charging. One needs to demonstrate that one can successfully sustain the large current required in the column.

5.2.6 Projection Ion Beam

Challenges include: the development of stencil masks as a production technology, beam interaction in the masks, and the whole issue of beam performance.

5.2.7 Projection X-Ray

Some of issues include masks, reflection lenses, debris in the laser-plasma sources, and resist technology.

5.2.8 Scanning Tunneling Microscopy

The major challenges for STM are: throughput, proximity effects, gap control, and tip longevity and control.

. Private discussion with Gene Fuller of TI.

. Marc D. Levenson, "Wavefront Engineering for Photolithography", Physics Today pages 28-36 (July 1993); and Garey E. Flores and Bruce Kirkpatrick, IEEE Spectrum pages 25-27 (October 1991).

Throughput is usually raised as a problem, but this is always in the context of the very high volumes of DRAM chips needed to amortize a state-of-the-art fab. These arguments should be re-analyzed in terms of cost effectiveness in a smaller product run, such as envisioned for random logic chips, ASIC, and in a cluster-tool environment.

Notes from private discussion with Gene Fuller of TI, who served as GCA program manager at SEMATECH for several years.

H. I Smith, Viewgraphs from presentation at Advanced Lithography Workshop at LaJolla, California July 14, 1993.

C. A. Mead (to be published).

G. A. Moore

Don K. Rose of Intel, Presentation to the Process Control Workshop in LaJolla July 16, 1993.

K. Sagara, T. Kura, S. Shukuri, J. Yugami, N. Hasegawa, H. Shrinriki, H.Goto,H. Yamashita, E. Takeda (Hitachi) in 1992 symp. on VLSI Technology (Seattle) Digest of Technical Papers, IEEE, New York (1992), p.10.

ADVANCED LITHOGRAPHY

T. McGill, D. Ferry, E. Hu,
R. Osgood, H. Ehrenreich

ADVANCED LITHOGRAPHY

BY

T. C. McGill, D. K. Ferry, E. Hu, R. Osgood, and H. Ehrenreich

PROBLEM

Lithography is the key to producing modern electronics. Each generation of shrinkage requires an advance in lithography. Optical lithography has been the dominant technique for years. It is important to determine what is limiting its development and to seek appropriate alternatives for the post-optical era.

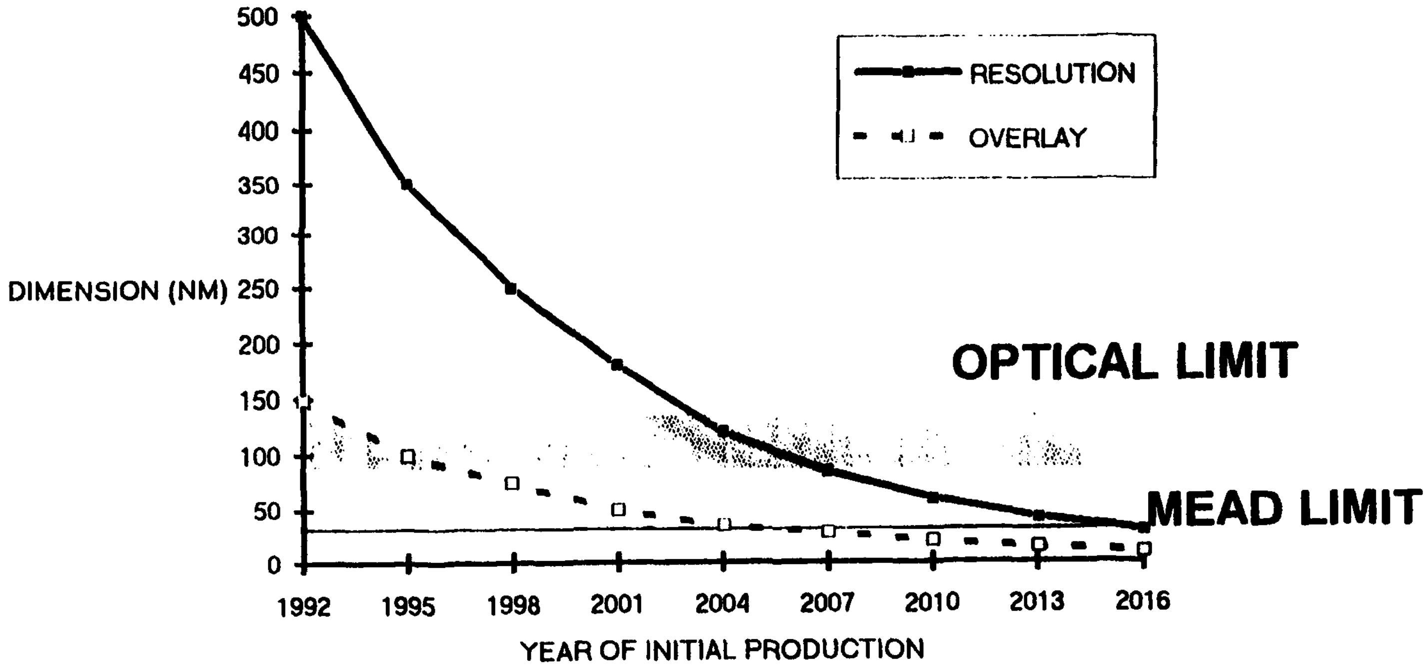
DoD Relevance

High performance electronics is essential to the modern military. Our ability to control our destiny in electronics depends on our ability to insure that we have access to the best lithographic tools available.

DS RC

LITHOGRAPHY REQUIREMENTS

PROJECTED DATE FOR INITIAL PRODUCTION



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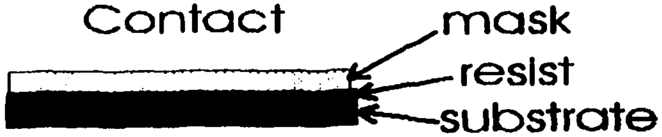
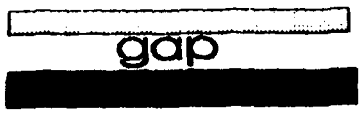
METHODS AND RESOLUTION LIMITS

Contact

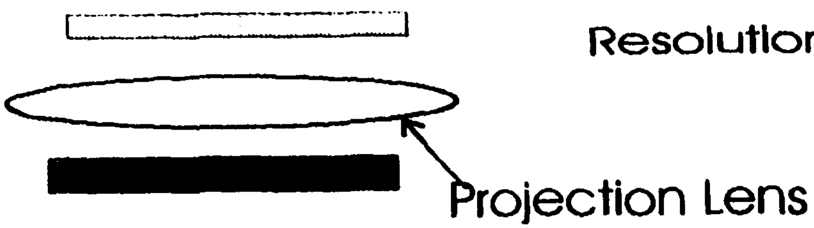


Proximity



$$\text{Resolution} = K(\text{gap} \times \text{wavelength})^{1/2}$$

Projection



$$\text{Resolution} = K \, \frac{\text{wavelength}}{\text{Numerical Aperture}}$$

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RESOLUTION LIMITS FOR PROJECTION OPTICAL

- i-line in Hg Source λ=365 nm
  - Projected Lower limit 261 nm
  - Phase-Shift Mask Lower Limit 250 nm
- KrF Excimer Laser λ=249 nm
  - Projected Lower limit 178 nm
  - Phase-Shift Mask Lower Limit 171 nm
- ArF Excimer Laser λ=193 nm
  - Projected Lower limit 138 nm
  - Phase-Shift Mask Lower Limit 132 nm
- F_2 Laser λ=157 nm
  - Projected Lower limit 112 nm
  - Phase-Shift Mask Lower Limit 108 nm

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ALTERNATIVES TO PROJECTION OPTICAL

- DIRECT WRITE E-BEAM
- PROXIMITY X-RAY
- CHARACTER BASED E-BEAM
- PROJECTION E-BEAM
- PROJECTION X-RAY
- PROJECTION ION
- SCANNING TUNNELING MICROSCOPY

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PERSONAL RANKING FOR POST OPTICAL ERA

- PROJECTION E-BEAM
- PROJECTION X-RAY
- PROJECTION ION-BEAM
- PROXIMITY X-RAY
- SCANNING TUNNELING MICROSCOPY

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SUMMARY

- OPTICAL LITHOGRAPHY IS LIKELY TO BE THE DOMINANT LITHOGRAPHIC METHOD WELL INTO THE NEXT CENTURY
- OPTICAL LITHOGRAPHY WILL STILL REQUIRE DEVELOPMENTS IN RESIST AND TECHNIQUES FOR DESIGNING PHASE-SHIFT MASKS PARTICULARLY FOR RANDOM LOGIC
- A NUMBER OF DIFFERENT TECHNIQUES EXIST FOR LITHOGRAPHY BELOW 0.18 μm
  - Proximity X-Ray
  - Projection E-Beam
  - Projection X-Ray
  - Projection Ion Beam
  - Scanning Tunneling Microscopy

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SUGGESTIONS FOR ARPA ACTION OVERALL

- MOVE PROGRAMS WITH HIGH LEVELS OF TECHNICAL READINESS TO ORGANIZATIONS CAPABLE OF PRODUCING SUBSTANTIAL MARKET AWARENESS
  - GCA/SVGL OPTICAL STEPPERS
  - PROXIMITY X-RAY
- ESTABLISH TECH BASE PROGRAM
  - PROVIDE TECH BASE FOR PUSHING OPTICAL TO THE ULTIMATE LIMIT
  - EXPLORE THE MOST TECHNICALLY PROMISING ALTERNATIVES FOR THE POST-OPTICAL ERA

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SUGGESTIONS FOR ARPA ACTION OPTICAL LITHOGRAPHY

- ESTABLISH A BASIC TECHNOLOGY PROGRAM IN OPTICAL LITHOGRAPHY
- SHORT WAVELENGTH RESISTS
- TECHNIQUES FOR DESIGNING PHASE-SHIFT MASKS FOR RANDOM LOGIC
- USE OF FOURIER OPTICS THROUGHOUT THE LITHOGRAPHY PROCESS

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SUGGESTIONS FOR ARPA ACTION PROXIMITY X-RAY

- FOCUS ON ESTABLISHING ITS APPROPRIATENESS AFTER THE OPTICAL ERA
- SMALL PROXIMITY GAPS
- STABILITY OF OVERLAYS
- MASKS TECHNOLOGY
- POINT SOURCES

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SUGGESTIONS FOR ARPA ACTION PROJECTION E-BEAM

- TEST FEASIBILITY OF SCAPEL (ATT) AND PREVAIL (IBM)
- ELECTRON OPTICAL SYSTEM FOR THIS APPLICATION
  - BEAM PROPERTIES
  - SPACE CHARGING
- THROUGHPUT
- MASKS FOR RANDOM LOGIC

DS RC

SUGGESTIONS FOR ARPA ACTION PROJECTION X-RAY

- FOCUS ON DEMONSTRATION OF FEASIBILITY
- REFLECTION OPTICAL ELEMENTS
- RESIST TECHNOLOGIES FOR THIS WAVELENGTH RANGE
- LASER PLASMA SOURCE
- MAKE SURE EFFORT HAS SERIOUS INPUT FROM A PRODUCT/MANUFACTURING POINT OF VIEW

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SUGGESTIONS FOR ARPA ACTION
PROJECTION ION BEAM

- CONCENTRATE ON DEMONSTRATING TECHNICAL FEASIBILITY
- STENCIL MASKS
- PERFORMANCE OF THE ION BEAM OPTICAL SYSTEM
- GEO/POLITICAL INTEGRATION OF THE PRODUCT

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SUGGESTIONS FOR ARPA ACTION
SCANNING TUNNELING MICROSCOPY

- UNIQUELY DIFFERENT CLASS
- LONGEST TERM
- ULTIMATE RESOLUTION
- MULTIPLE TIPS FOR THROUGHPUT
- “RESIST” PROCESS

ADVANCED LITHOGRAPHY

ARPA

ADVANCED LITHOGRAPHY

Workshop Coordinator: Thomas C. McGill

July 13, 1993

1:00 pm	Workshop Purpose, Ground Rules and Agenda, Sven Roosild (ARPA), Tom McGill (DSRC/Caltech)
1:30 pm	"Optical Lithography," Gene Fuller (TI)
	Direct Write E-Beam Lithography
2:30 pm	"E-Beam Lithography," Hans Pfeffer (IBM)
3:20 pm	"Novel Approaches to Improve E-Beam Throughput," N. McDonald (Cornell)
3:35 pm	"Direct Write E-Beam," M. Lepselter (Lepton Corp.)

July 14, 1993

8:00 am	"Proximity X-Ray", Hank I. Smith (MIT)
9:00 am	"SCALPEL", Steven Berger (ATT Bell)
10:00 am	Break
	Ion Beam Lithography
10:15 am	"Overview of Project", Hans Loschner (IMS GmbH)
10:25 am	"Technical Issues", G. Stengl (IMS GmbH)
11:00 am	"Technical Issues", John Melingalis (MIT)
11:15 am	"Projection X-Ray", David Widmer (ATT Bell Labs)
12:15 pm	Lunch
1:00 pm	"STM", Fabian Pease (Stanford University)
2:00 pm	General Discussion

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WHITHER REAL-TIME PROCESS CONTROL

E.L. Hu and G. Larrabee

EXECUTIVE SUMMARY

Objective of the Workshop

The implementation into manufacturing of each successive device generation has been accomplished against a background of continually increased challenges in processing and economic viability. The need to maintain resolution of feature sizes well below 0.25μm, and process uniformity over wafer sizes greater than 8 inches in diameter will push the capabilities of open-loop processing. The need to quickly ramp up the process learning curve, achieving cutting-edge manufacturing costs by the highest equipment utilization and highest product yield will require enhanced capabilities of processing equipment. Real-time process control strategies will be especially pertinent to flexible microelectronics manufacturing, suitable for rapid turnaround of a multiplicity of small product quantities. In recent years, substantial progress has been made in the identification and utilization of appropriate sensors, and in the construction of pragmatic and effective process *and* control models. Moreover, these components have been successfully integrated within the ARPA/Air Force/TI MMST program, which has demonstrated the very impressive cycle times of 3 days for the production of 0.35μm CMOS chips.

The goal of this workshop was to explore the necessary next steps to bring real time process control from outstanding proof-of-concept into real manufacturing. We attempted to construct a full and realistic view by understanding not only the possibilities and potential of real-time process control, but as well by understanding the outstanding issues to be addressed, as presented by both an equipment manufacturer and by a large commodity manufacturer utilizing single-product, "rigid" fabs.

DoD Relevance

As has been stated in other workshops, modern microelectronic integrated circuits are crucial to the performance of modern smart weapons systems, to communications, and to command and control support systems. DoD commands a fraction (10%) of the total IC market, and its needs more closely fit within the operation of an ASIC manufacturer rather than a large commodity manufacturer. That is, although DoD requires rapid prototyping of state-of-the-art IC's for quick time to market, and access to a variety of part types, the total quantities required may be modest. This requires flexible, intelligent manufacturing capabilities, but such strategies will be widely accepted only as equipment that supports their implementation is available under the same quasi-"off the shelf" basis as current equipment. The same guarantees of process robustness, and equipment reliability at reasonable cost must pertain. However, the economics used by equipment vendors is largely determined by the commodity market which operates on an economy-of-scale model.

Furthermore, the acceptance of real-time process control strategies has implications and benefits for a broader class of technologies of interest to DoD, e.g. the manufacture of high performance materials such as sapphire fibers or diamond substrates. In addition, the development of sensor-based monitoring, and of enhanced process and process equipment understanding should have important benefits for environmentally responsible manufacturing strategies.

Scientific and Technological Summary

Substantial progress has been made in the utilization of sensor-driven process control for microelectronics manufacture. Open-loop monitoring, such as used in real-time ellipsometry to monitor etch rates (of silicon) has shown clear advantages over simple "timed" etches in being able to drive the process to the target values. Such simple approaches, even without implementation of a control strategy, can compensate for variations in materials and process parameters, including "first wafer" effects. Effective control models and strategies have been been implemented even for the apparently complex set of Rapid Thermal Processes. In this case, not only was the process driven to the target value, for example, achieving impressive run-to-run reproducibility of deposited polysilicon, but even longer range benefits were realized. The determina-

tion of the appropriate control strategy identified the appropriate, critical parameters to be controlled *and* provided input to the design of the equipment. Progress has also been made in the areas of process modelling and even process *equipment* modelling, most notably in thermal and fluid-flow problems. An outstanding demonstration/validation of real-time process control strategies is to be found in the successes of the MMST program at TI, which provided fully integrated processing to achieve a record 3-day cycle time for IC manufacture.

These successes notwithstanding, full scale implementation of real-time process control for microelectronics manufacturing will not take place until suitable "off-the-shelf" equipment is available at reasonable cost, with the necessary complement of sensors and of control software. Major microelectronics equipment vendors are in turn necessarily sensitive to the market demands of their largest customers: manufacturers such as Intel, which utilize single-product, "rigid" fabs. Intel's manufacturing strategy includes early (several generations in advance) identification and development of processes on existing equipment, locking-in on processes during manufacture and requirement of absolute stability of the fully characterized processes. The introduction of perturbations to process or equipment reliability is therefore uneconomic and unacceptable. Possible beneficial insertions might be simple, low-cost enhancements on *existing* equipment that would shorten the process development time or similarly might decrease equipment maintenance and down-time (and ultimately eliminate the need for equipment "seasoning"). Use of low-cost sensors in an open-loop, monitoring scheme that can effectively drive the process to target values is a viable initial strategy. It is interesting to note that Intel's experience has been that software reliability ("lock-up") is the biggest equipment problem, after defects. This is clearly an important issue in the introduction of additional software to enable sensor-based supervisory control of processes.

Conclusions

Real-time process control strategies have already demonstrated impressive enhancements in process capability. Longer range benefits will be realized as these strategies are more widely implemented with further development of *in situ* sensors, signal processing techniques, and process models. Better understanding of the processes will lead to better design of processing equipment, a faster progression up the process learning curve and more efficient equipment

utilization. The acceptance, need and incorporation of such strategies will proceed at different rates in different areas of microelectronics manufacturing, but the real implementation into manufacturing requires that compatible, low cost equipment be available "off the shelf". This will require the availability/ development of robust, low-cost sensors, reliable control software and standard interfaces for both hardware and software.

Opportunities for ARPA

Real-time process control is on the threshold of real integration into full-scale microelectronics manufacturing. The most critical step is ensuring the availability of compatible, sensor-clad, low cost, reliable processing equipment as "off-the shelf" items.

1. ARPA's new program that works with equipment manufacturers to bring to market equipment from the MMST program that will enable real-time process control is the exact, appropriate next step. As a first step, such equipment could simply utilize, initially, low-cost, robust sensors running open-loop, but which could significantly enhance process performance by driving the process to target values.

2. To be econonomically available to the broad range of equipment manufacturers, standards for sensor interfaces and software must be defined and enforced. This is largely the role of SEMI, aided by SEMATECH; ARPA has numerous programs which are exploring process control strategies at various levels, and so can ensure, where appropriate, that these standards are observed.

   In addition, these strategies should be incorporated in ARPA's existing programs, where appropriate. For example, real-time process control, and its ancillary benefits of better process understanding and improved equipment design, will have enormous benefits in implementing environmentally responsible manufacturing.

3. Reliable, fault-tolerant software will be a critical need; the incorpora-

tion of real-time process control capabilities into equipment will aggravate software reliability problems. Fault-tolerant software for high performance computing is an established area of activity. Some examination should be made of appropriate fault-tolerant strategies for controlling software in this context.

WHITHER REAL-TIME PROCESS CONTROL FOR MICROELECTRONICS MANUFACTURING?

E. Hu and G. Larrabee

WHITHER REAL-TIME PROCESS CONTROL FOR MICROELECTRONICS MANUFACTURING?

E. HU AND G. LARRABEE

Objective

- Identify and "attack" impediments to implementation of real-time process control in microelectronics manufacturing.

Relevance to DoD

- Modern microelectronic integrated circuits (ICs) are crucial to the performance of modern smart weapons systems, communications and to command and control systems.

- The DoD requires rapid protyping state-of-the-art ICs for quick time to market and access to a variety of part types.

  ⇒ Requires flexible intelligent microelectronics manufacturing (FIMM), hence real-time process control

- Real-time process control has implications and benefits for a broader class of important technologies for the DoD

  ⇒ Manufacture of sapphire fibers and diamond substrates
  ⇒ Environmentally responsible manufacturing

Summary

- Benefits of real-time process control demonstrated by MMST successes:
  - 3-day cycle time
  - 100% single-wafer processing
- Progress being made in use of sensors, control and process models
- Need for, and implementation of real-time process control will differ according to manufacturing need

Conclusions

- Real-time process control strategies have demonstrated impressive enhancements in process capability

- Further development of *in situ* sensors, signal processing techniques and process models will enhance more wide-scale implementation in manufacturing

- Require "off-the-shelf," low-cost equipment with embedded real-time process control

    - low-cost sensors
    - reliable control software
    - standard interfaces for both hardware and software

Opportunities for ARPA

- The ARPA program to bring MMST equipment innovations to market is the exact appropriate next step
- ARPA should support and utilize SEMI (SEMATECH development of standards (interfaces, software)
- Real-time process control should be an integral part of ARPA environmentally responsible manufacturing programs
- Reliable fault-tolerant software will be a critical requirement for process control software

WHITHER REAL TIME PROCESS CONTROL MICROELECTRONICS MANUFACTURING

Workshop Organizer: Evelyn Hu
Workshop Organizer: Graydon Larrabee

July 16, 1993

8:00 am	Workshop Overview, Evelyn Hu (DSRC/UCSB)
8:30 am	"Microelectronics Manufacturing Science and Technology (MMST) Process Control Successes," Bob Doering (TI)
9:15 am	"Real Time Process Control in Manufacturing — An Equipment Maker's View," Eric Nering (LAM)
	"Real Time Process Control — Technology That is Being Proven in the Lab Today," Michael Elta (University of Michigan)10:15 am Break
10:45 am	"Real Time Process Control in Manufacturing—A device manufacturer's view," Don Rose (Intel)
12:00	Lunch
1:00 pm	"SEMATECH, SEMI and SIA Microelectronic Manufacturing Process Control Road Maps," David Partington (SEMATECH)
	"Ongoing SEMATECH, SEMI and SIA Process Control/ CIM Activities and Road Maps," Alan Weber (SEMATECH)
2:00 pm	Discussions on "Whither Real Time Process Control for Microelectronics Manufacturing"

REAL TIME PROCESS CONTROL FOR MICROELECTRONICS MANUFACTURING

July 16, 1993

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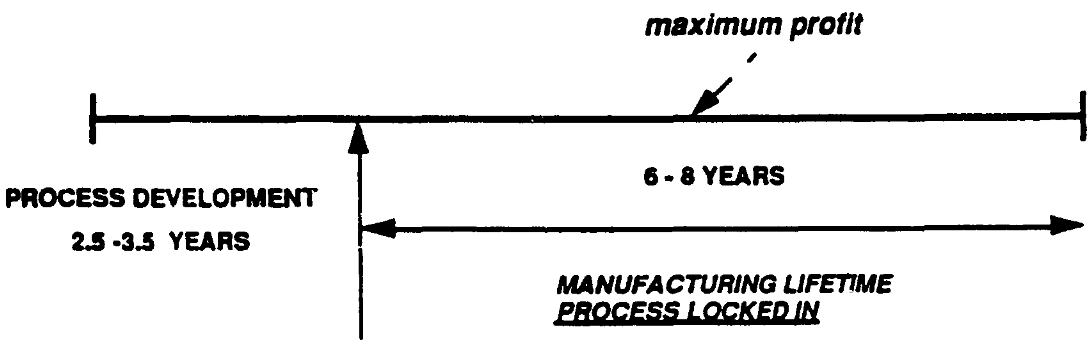
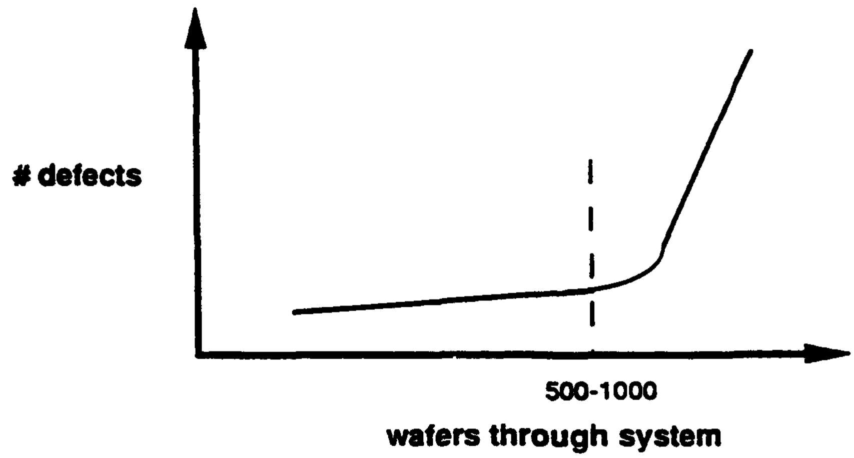
APPENDIX

Intel's Relentless Pace to Market

An interesting perspective on the a manufacturing strategy was given by Don Rose of Intel. A typical manufacturing cycle is represented by the time-line below, where concerted process development is initiated 2.5 - 3.5 years before ramping into full manufacturing production. Process development is carried out *on the equipment* which will be used in manufacturing. After the development phase is concluded, the processes are locked-in and not be changed, even if more attractive process alternatives may have developed in the interim.



This strategy means that decisions on equipment purchase must be made well in advance of the actual usage of equipment in production; moreover, Intel utilizes ~ 70% of the equipment for the next generation production, so choices on equipment are indeed locked-in early. Economics dictate that equipment up-time and utilization be kept as high as possible; Rose quoted values of 90% up-time and 70% utilization on product wafers. Because the processes utilize existing equipment, whose process performance must be as reliable as possible, Intel chooses to use extremely careful and thorough characterization of processes rather than sensor-based monitoring of processes. Such characterization provides data such as the curve below, which is used to determine the number of wafers that can be continuously run (for each machine) before the equipment is shut down for maintenance, cleaning and seasoning.



Such an approach at present is preferable to shut-downs based on sensor-monitoring of the equipment, since no adequate correlations could be established between particles monitored by in-line sensors and particles actually found on the processed wafers. Moreover, the addition of sensors and ancillary software may add yet another weak link in the chain of reliability of the equipment. One can envision substantial benefits to this mode of manufacturing by

(1) Shortening the process development time

(2) Eventually aiding in minimizing machine down-time for maintenance and seasoning.

In any case, the introduction of process control strategies here must be done "seamlessly" through the availability of reasonably priced, reliable equipment that will provide enhanced process capability. Since "rigid" fab manufacturers such as Intel provide a substantial share of the market for semiconductor processing equipment, this is clearly an area to be targeted, although the present need for intelligent process control may not be as critical as it is for smaller volume chip (ASIC) manufacturers.

ENVIRONMENTALLY RESPONSIBLE MANUFACTURING

Graydon Larrabee and Robert Rapp

EXECUTIVE SUMMARY

Workshop Objective

The processing of most feed stocks and the manufacture of components and complete systems, ranging from unfinished steel to silicon wafers to computers, generally requires huge amounts of water, process gases, chemicals, hazardous materials, fuels and electrical energy. The practices of the recent past for disposal and landfilling of waste products by standards marginally acceptable to government regulation has proven to be expensive both to the environment and to industry, so that the command-and-comply strategy has not been effective.

In the global economy of the 1990s, environmentally responsible manufacturing will be mandatory just to compete, and US companies are maintaining the same environmental standards abroad as at home. Industries cannot play catchup to the increasingly strict regulations, but can find it to their economic advantage to lead in applying the three R's: reuse, remanufacture, and recycle, to achieve a "cradle-to-grave" accountability. This workshop was designed to address the issues and specific technical procedures involved with environmentally responsible manufacturing. The roles of the government generally and the DOD specifically in effecting pollution prevention and resource conservation in manufacturing were explored.

Relevance to DoD

As the largest economic unit in the country, the US government is the foremost purchaser of manufactured products, which indeed are subject to governmental health, environmental, and safety regulations. The DOD is aware and concerned about the creation and/or perpetuation of environmentally hazardous conditions that may have been established by the DOD or its contractors as a consequence of the manufacture, maintenance and use of military

equipment and weapon system components. Likewise, the industrial sector feels increased market pressures from both domestic regulatory constraints and growing foreign legislative and "take-back" policies. Often changes in processes, materials or procedures, or the reuse and recycling of components or materials, leads to both lower costs and improved products, with the avoidance of costly fines, delays and bad publicity. As an inverse spin-off from industrially developed processes or products to absorb hazardous gases, filter solids or clean surfaces, etc., the military might find applications in its military equipment and processes, e.g. gas masks and painting airplanes.

Throughout its wide system of shops and facilities, the DOD is itself involved in repair and manufacturing, so the life cycle design which guides the US industry could also be adopted by the DOD, to gain the same advantages. To minimize the cost for the purchase of improved manufactured products, the DOD could require certain standards, and offer certain guidance, to the industrial manufacturers of military equipment and weapons systems. Other government agencies such as NSF and the Commerce Department could sponsor research and economic studies to support the integration of the ecofactory with life cycle design into flexible intelligent manufacturing, to achieve a "cradle-to-grave" accountability. These agencies could also take a lead role in providing educational modules which explain these concepts.

Scientific and Technical Summary

The workshop identified a number of non-obvious industrial practices which not only led to monetary savings, but also to a conservation of resources and the prevention of pollution:

1. Design for disassembly with recycle of components or materials. Used modules with residual life, e.g. electromechanical systems recovered from a copying machine, could be reused, e.g. in a printer. For ease in reuse and recycling, a minimum number of different materials should be selected, i.e. a limited choice of plastics, glass, electronics and alloys which should be coded, preferably by molded labels. The use of adhesives and pasted labels should be minimized to facilitate disassembly and recycling. Often special tools or robots need to be designed for a specific disassembly job.

2. The "takeback" and leasing of manufactured products, while perhaps instigated for environmental reasons, could provide the US manufac-

turer with a revolutionary advantage in global competition. By assuming a continuing responsibility and accountability for a product, the infrastructure to provide prompt service and product upgrading should lead to repeat (or captive) customers and a larger market share. Generally, the upgrading of products is an evolutionary process achieved by incremental improvements. The takeback and leasing of products leads to an opportunity for upgrading components, and to a greater variety of products evolving from one product base. Customers want a reliable product at a good price with the expectation of good service; they do not care whether the product is comprised of reused components or recycled materials. Some components, e.g. the toner cartridges for copiers or FAX machines, can be returned, refilled and reused. A leased computer can be upgraded as improvements are made possible.

3. As one goal of responsible manufacturing, the industry must attempt also to produce products exhibiting a minimum demand on the environment. Their products should be specifically rated with respect to energy consumption, dispersion of hazardous ingredients, CO_2 release, and other risks. For example, a "green computer" would consume little electrical energy in use, with a provision for "sleeping" when not in use. In their purchases of equipment, the government and the DOD could require such labeling of specifications, and purchase accordingly.

4. To effect environmentally responsible manufacturing, the senior management must be involved as process enablers. Generally, the number of employees may increase, although money is saved overall. The corporate decision to develop planned roadmaps for the conversion to more environmentally responsible manufacturing will depend upon the existence of cost models and data banks to evaluate such changes. There is, however, a need for research and development in topics of pollution monitoring and abatement, such as absorption of specific hazardous gases, the cleaning of surfaces, development of species-specific sensors, filtration of liquids, etc. Each of the several companies which were represented at the workshop, namely Texas Instruments, Xerox, Digital Electronics, Martin-Marietta and

Sematech, have experienced financial savings by the introduction of ecofactory concepts.

5. General information about money-saving, environmental manufacturing procedures is often shared, even among competitors within a commercial sector, through publications, presentations, meetings and professional or trade societies. Such responsible actions should be encouraged. However, companies will develop proprietary, non-patented positions for certain critical processes which will be held secret from the competition. At the moment, Universities do not seem to be participating adequately in instilling an environmental awareness or technical expertise in their students. Part of the problem lies in the lack of knowledge and appropriate educational materials for the faculty, in addition to the many other demands on the University curriculum.

Perhaps the governmental funding of research in pollution abatement and responsible manufacturing is also not adequate.

Conclusions and Observations

Environmentally responsible manufacturing must incorporate the concepts of Life Cycle Design (LCD) or Design for the Environment (DFE): design for disassembly, material selection for recycle, life extension through reuse, remanufacture and product conversion. In the factory, LCD must account for energy consumption during manufacture, and pollution abatement by the minimal use with recycle of chemicals, water, and gases, and an avoidance of hazardous components. After manufacture, the industry must participate in the take-back and leasing of products. The associated servicing and upgrading of products could lead to a significant advantage for US manufactures in global competition. In service, these products should operate with a minimal use of energy and a minimal release of CO_2 and other environmental hazards.

Certain support technologies need further development for the broad realization of environmentally responsible manufacturing:

1. Disassembly, including design for disassembly, identification and separation of materials, recycling of advanced materials and composites, and automated (robotic) disassembly.

2. Ecofactory (embedded in Flexible Intelligent Manufacturing), including real-time process control, minimized consumption of energy and chemicals, and elimination of emissions and solid wastes.
3. Data Bases and Cost Models, including those evaluating the environmental impact of chemical and materials choices, and ratings for energy and CO_2 and other releases by manufactured products.
4. Education, including new knowledge to drive new technology development, and the preparation of educational modules for teaching and training engineers, technicians and scientists.

The successful modern industries have found an advantage in staying ahead of regulated constraints. Their environmental responses have led to saving money, even when the factory is offshore. Some of this experience is shared within an industrial sector, but the expertise and educational materials needed for participation by the Universities are not available. The DOD can effect environmentally responsible manufacturing by specifying certain manufacturing standards and procedures, and by providing public information about environmentally safe processes, materials, and procedures.

ENVIRONMENTALLY RESPONSIBLE MANUFACTURING

G. Larrabee and R. Rapp

Objective

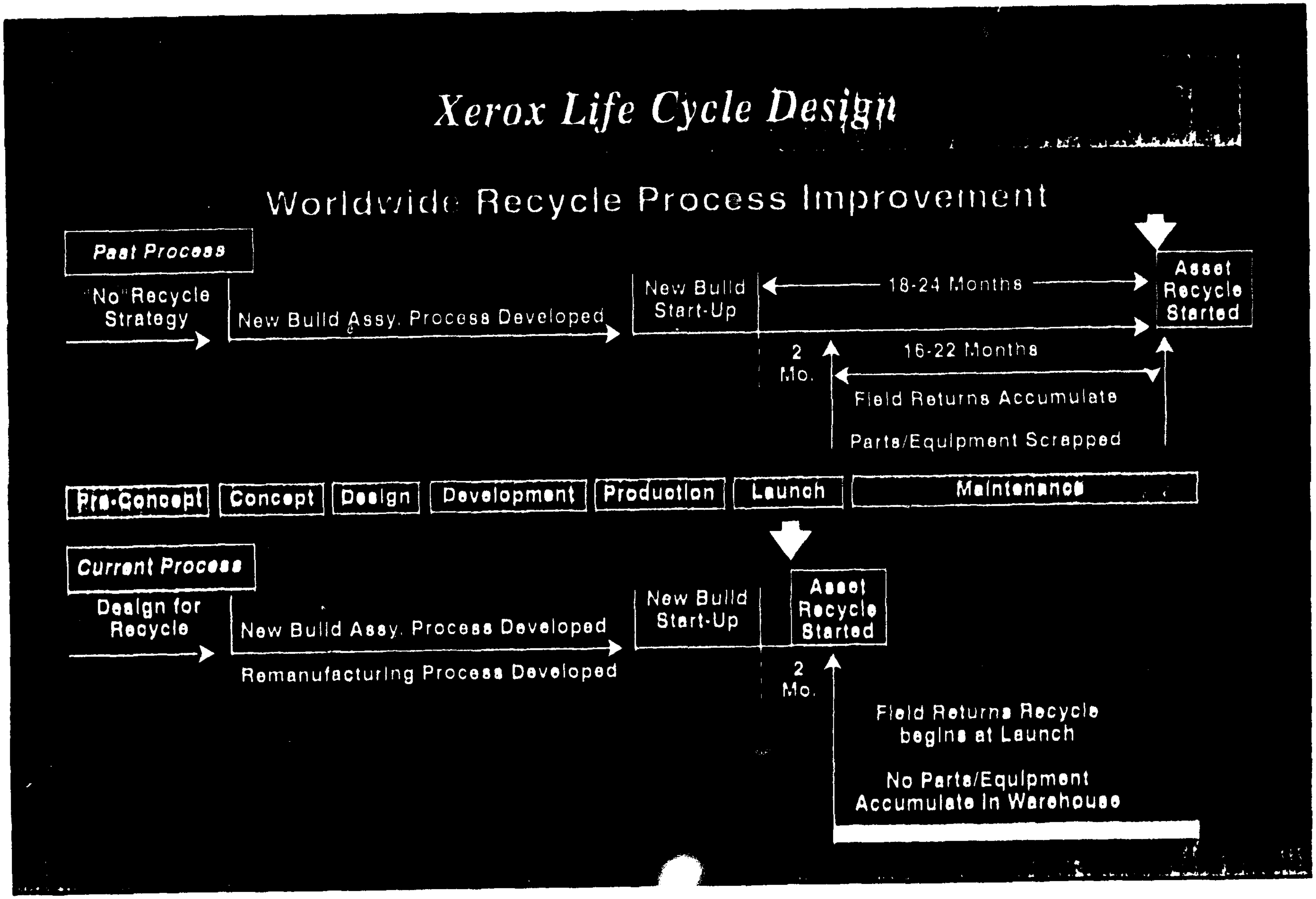
- The workshop was designed to address the issues surrounding environmentally responsible manufacturing and identify what technical choices are available.

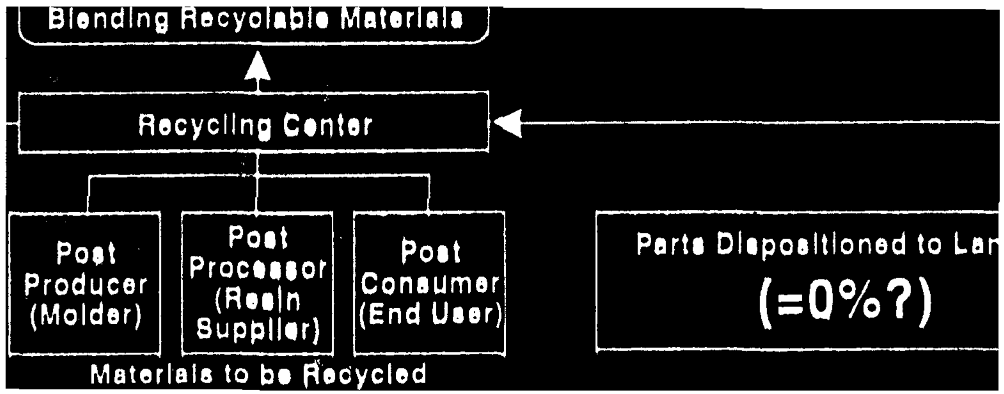
Relevance to DoD

- DoD and its contractors must address the consequences of manufacture, maintenance and use of military equipment and weapons systems.
- American industry must compete in a global economy in the 1990s and beyond.
  - Environmentally responsible manufacturing will be mandatory just to compete.
  - Command-and-comply strategy has not worked.
  - Industry must take the lead.

Life Cycle Design (LCD) or Design for the Environment (DFE)

- Manufacturers will take total responsibility for their product from "cradle to grave"
- Life cycle design plays an overwhelming role and will comprehend:
  - Disassembly
  - Material selection and recycle
  - Life extension through reuse
  - Remanufacture and product conversion
- Life cycle design comprehends manufacturing issues:
  - Energy consumption
  - Chemicals usage and recycle
  - Waste generation
- New concepts evolve:
  - Product leasing in place of buying
  - Manufacturing raw materials leasing, e.g. plastics
  - Product packaging delivers new product and returns leased product


Xerox Life Cycle Design
Worldwide Recycle Process Improvement
Past Process
"No" Recycle Strategy
New Build Assy. Process Developed
New Build Start-Up
18-24 Months
Asset Recycle Started
2 Mo.
16-22 Months
Field Returns Accumulate
Parts/Equipment Scrapped
Pre-Concept
Concept
Design
Development
Production
Launch
Maintenance
Current Process
Design for Recycle
New Build Assy. Process Developed
Remanufacturing Process Developed
New Build Start-Up
Asset Recycle Started
2 Mo.
Field Returns Recycle begins at Launch
No Parts/Equipment Accumulate In Warehouse


Blending Recyclable Materials
Recycling Center
Post Producer (Molder)
Post Processor (Resin Supplier)
Post Consumer (End User)
Materials to be Recycled
Parts Dispositioned to Lan
(=0%?)

The Ecofactory Embedded in Flexible Intelligent Manufacturing

- Design technology
  - Maximize product recycle and minimize manufacturing environmental impact
- Production technology
  - Environmentally responsible production processes
- Dismantling technology
  - Intelligent, automated dismantling
- Reprocessing technology
  - Produce materials, modules and products that meet “new” product specifications

Support Technologies that Need Attention

- Disassembly
  - Design for disassembly
  - Dismantling, identification and separation of materials
  - Advanced materials and composites recycling
  - Automated disassembly — robots
- Ecofactory — Embedded in Flexible Intelligent Manufacturing
  - Real time process control
  - Minimized energy and chemical consumption e.g., new cleaning technologies
  - Eliminate emissions and solid wastes
- Education
  - New knowledge to drive new technology development
  - Trained engineers and scientists
  - Preparation of education modules for teaching and training

Support Technologies that Need Attention (Contd.)

- Data bases and Cost Models
  - Cost models to evaluate environmental impact in manufacturing
  - Data bases for environmental impact of chemical and materials choices
  - Ratings for energy consumption and CO_2 emission

Observations

- Pressure from American consumers and legislation enacted in foreign countries will drive industry and the DoD to embrace environmentally responsible manufacturing.
- Economics can be very favorable — Xerox estimates savings of $50M in the first year.
- United States is 2 to 3 years ahead of Japan. European consumers more "green-oriented."
- University generation of new technologies is not happening — it is not clear why, the NSF program is clearly inadequate.

Conclusions

- In the 1970–80s, quality was the driver for world class, global companies

  In the 1990s and 2000s, environmental responsibility will be the metric

- New technologies will be needed for environmentally responsible manufacturing
  - Disassembly
  - Ecofactory
  - Education
  - Data bases and cost models

Summary

- American industry and the DoD must implement environmentally responsible manufacturing
  - "Cradle-to-grave" accountability
- Ecofactory concepts will need to be integrated into flexible intelligent manufacturing
  - Life cycle design
- Support technologies needed include:
  - Disassembly
  - Ecofactory
  - Education
  - Data bases and cost models
- American industry must take the lead

ENVIRONMENTALLY RESPONSIBLE MANUFACTURING

Workshop Organizer: Graydon Larrabee
Workshop Organizer: Robert A. Rapp

July 19, 1993

8:00 am	Workshop Overview, Graydon Larrabee (DSRC)
8:30 am	"Manufacturing Design for Product Take-back, Disassembly, Reuse and Recycle," Jack Azar (Xerox)
9:20 am	"Green Workstation Manufacturing Analysis/New Technology Needs," Bob Ferrone (DEC)
10:10 am	Break
10:40 am	"Environmentally Responsible Manufacturing in the Aerospace Industry," Jack Snyder (Martin Marietta)
11:30 am	"Implications of Environmental Activities in Europe and Japan," Deanna Richards (National Adademy of Engineering)
12:00 Noon	Lunch
1:00 pm	"Will American Universities Conceive and Demonstrate the Requisite Tools and Technologies?", Henry McGee (NSF)
1:45 pm	"SEMATECH and SIA Environmentally Responsible Manufacturing Roadmaps," Ray Kerby (SEMATECH)
2:30 pm	Discussions: NEXT — What, When, Who

ENVIRONMENTALLY RESPONSIBLE MANUFACTURING

July 19, 1993

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LIFE EXTENSION OF AGING AIR-CRAFT SYSTEMS

B. Budiansky, A. G. Evans, J. W. Hutchinson, A. H. Heuer, R. Rapp, J. C. Williams

EXECUTIVE SUMMARY

Workshop Objective and Relevance

A large fraction of the military and commercial aircraft fleet has been in use for decades and, in some cases, has exceeded its originally designated design life. Yet, it is not economically realistic to replace the overaged airplanes and helicopters. The consequence is a need to address simultaneously two aspects of the life of aging aircraft:

(i) Extend reliably predicted life by improved understanding and analytical capability as well as improved data records and stress histories.

(ii) Extend actual longevity of aging systems through improved diagnostics in conjunction with environmental protection, repairs, replacements and reinforcements.

There are activities funded by the FAA, NASA, the Air Force and the Navy attempting to identify the real problems and to find solutions. However, it was considered necessary to examine the phenomenon broadly in order to assess the extent to which the problems had been correctly identified and to judge whether strategies were in place to understand them and to reach solutions. Problems in both military and civil aviation, including air frames and engines of airplanes and helicopters, were surveyed.

Scientific and Technological Issues

The four prevalent themes in all of the aging aircraft activities are (i) fatigue, (ii) corrosion, (iii) diagnostics and (iv) active systems. Among these four themes are several issues: sensors, imaging of defects, signal analysis, crack growth modeling, and probablistic analysis. There are special problems in engines associated with new higher temperature goals.

There are also strikingly different levels of sophistication presently utilized by the different groups working on airframes, helicopters and engines. These differences have arisen because of different performance requirements and historical design strategies. Increased interaction among these groups in the future would have some obvious immediate benefits.

It is clear that there is inadequate integration of the four themes. Such integration is needed to relate the diagnostics obtained from the sensors to the fatigue life and the corrosion damage. It is proposed that a new discipline of prognostics be created.

Fatigue

There is one overarching issue concerning fatigue and corrosion fatigue. In many cases, the stress and temperature histories experienced by critical components have been poorly predicted at the design stage. Consequently, the fraction of fatigue life actually used differs from that predicted by design calculations. Real time sensing of stress and temperature at distributed locations would, in principle, allow continuous updating of the residual life and residual strength. Such sensor development and implementation is strongly recommended.

Another question concerns the role of multiple site damage (MSD) on the residual life and strength. This question is being addressed (probably adequately) by the FAA, NASA and the Air Force. DSRC members are already involved.

The basic mechanisms of fatigue crack initiation and growth are still not fundamentally understood, despite decades of research. Moreover, there is even less understanding about the mechanisms of corrosion fatigue. The consequence is a complete reliance on experimental measurements e.g. Paris Law data for crack growth. An enlightened approach to the fundamentals of fracture, fatigue and corrosion fatigue is urged, with a new impetus relevant to aging aircraft. Otherwise, enormous amounts of data will be needed (perhaps in new crack growth regimes) to permit reliable prediction of fatigue life.

Corrosion

There are numerous corrosion problems in airplanes and helicopters which usually arise when electrolytes (such as sea water) accumulate in regions of the fuselage. One example is the problem that arises because the combinations of materials used at fastener connections are inherently prone to corrosion upon their galvanic coupling. There is a particular problem where composite and Al alloy elements are attached to each other by Ti fasteners. The corrosion fundamentals are well-known. Strategies for solving the problems have been proposed, but the extent to which they have been implemented is not clear.

By assuming that the basic choice of materials cannot be changed (to materials intrinsically less proned to corrosion), two strategies have been contemplated. (i) Coatings or interlayers have been used inside the fasteners which are either protective, sacrificial, or electrically insulating. This strategy has not been successful, because the coating is rapidly abraded around the fastener in service. (ii) A polymer-based coating has been used to exclude the electrolyte from the fastener. Some success has been achieved using this approach.

The corrosion prevention/protection strategy is an open challenge. (Coatings for stress corrosion protection are being developed by the Navy.) New concepts are also being actively sought both by the Navy and by the commercial airframe manufacturers.

Diagnostics

The diagnostics being used are drastically different for engines, airframes and helicopters. These differences reflect the complexity of the components, their accessibility and the opportunity to dissemble for inspection. There are two general types of diagnostics. (i) Continuous sensing of displacements, acceleration or strains, and (in some cases) temperatures. (ii) Non-destructive detection of flaws, defects, corrosion pits, etc. at periodic inspection intervals. An optimum diagnostic method would involve both.

The most sophisticated use of continuous monitoring has been with helicopters. The best technology has been developed in Europe, particularly in the U. K. This situation has arisen for three reasons: (i) Helicopters have stress histories that change drastically and unpredictably during use,

because of changes in vibrational spectra. (ii) There are many components on helicopters which are difficult to disassemble, and so non-destructive inspection of all parts for individual flaws is not feasible. (iii) There is a recent history of helicopter crashes because of fatigue and corrosion; these have been highly publicized in the U.K.

The most sophisticated European monitoring systems consist of accelerometers placed at numerous locations. This serves two purposes: (i) The dynamics of the helicopter can be adjusted to minimize vibration during a typical flight trajectory. This reduces stress and extends the actual fatigue life. (ii) Signals from "failed" regions can be distinguished out of the spectrum. Such "failures" include broken gear teeth, bolts, etc. A proposed use of this method for fatigue crack detection is considered questionable.

In addition to transferring the European technology to the U. S., and using it in other sectors, there are some clear opportunities for improved sensing and signal analysis.

Non-destructive inspection of components for individual flaws and inclusions by eddy current and ultrasonic methods is a well-developed and continually evolving technology. Far reaching strategies for advanced imaging systems are used for periodic inspection of engine components in order to detect small flaws. In this case, complete disassembly is required and routinely done so that all parts can be comprehensively inspected. There is one open issue: the probabilistics of flaw detection (POD) require input from fundamental analysis of NDI methods.

The applications of NDI methods to airframes and helicopters involve different challenges. For the former, large area scanning is involved and, for both, there are regions inaccessible to conventional sensors. The detection of sub-surface damage, particularly with composites, represents another challenge. There is a major opportunity here for innovative sensors, imaging methods and signal analysis.

Active Systems

The use of active systems has the potential for reducing stress and extending the fatigue life. The major opportunities are with helicopters which incur large amplitude vibrations. Already, Westland in the U. K. has an

active system, using accelerometers and hydraulic actuators, with demonstrated improvements in vibration amplitude. Programs on smart systems already underway might be steered toward enhancing life expectancy of new systems.

Integration and Prognostics

There has been minimal effort at developing relationships between fatigue (or corrosion fatigue) performance and the information obtained from either continuous sensing or NDI. An exception is fatigue life prediction based on the detection of relatively large cracks in airframes and engine components. There is a major opportunity to combine advanced concepts in fatigue models with new sensors and imaging concepts, having the objective of relating sensor diagnostics to residual fatigue life and residual strength. Probabilistics are integral to this prognostics methodology.

Engines

The engine industry has the most sophisticated use of fatigue analysis, NDI and probabilistics. There are no obvious requirements for life extension strategies relevant to existing engines. A possible exception is the improved detection of "hard _SYMBOL 97 \f "Symbol"§" inclusions in Ti alloys.

The major issues relate to life analysis for future generations of engines. These engines will operate at higher temperatures for considerably longer times and will use metal and ceramic matrix composites. At higher operating temperatures, new damage and fatigue mechanisms are incurred. For example, hold time phenomena arise in Ni alloys. These are related to environmental acceleration of damage mechanisms. There is no commonly accepted lifing strategy when such mechanisms operate. Similarly, lifing strategies for MMCs and CMCs are not established.

Conclusions

There is a major opportunity for an integrated program that brings together new concepts in sensors with mechanistic models of fatigue to create a prognostics discipline, relevant to life extension in aging aircraft.

A feasibility study is needed to establish whether small fatigue cracks in helicopter rotor heads have any influence on the flight dynamics.

The use of retrospective fracture mechanics on aircraft components is strongly urged, as also recommended in 1992.

Coordination among the various efforts is needed, perhaps with the assistance of a "Blue Ribbon Team".

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

B. Budiansky, A. G. Evans,
R. Crowe, A. H. Heuer,
J. W. Hutchinson, R. A. Rapp
and J. C. Williams

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

RELEVANCE TO DOD

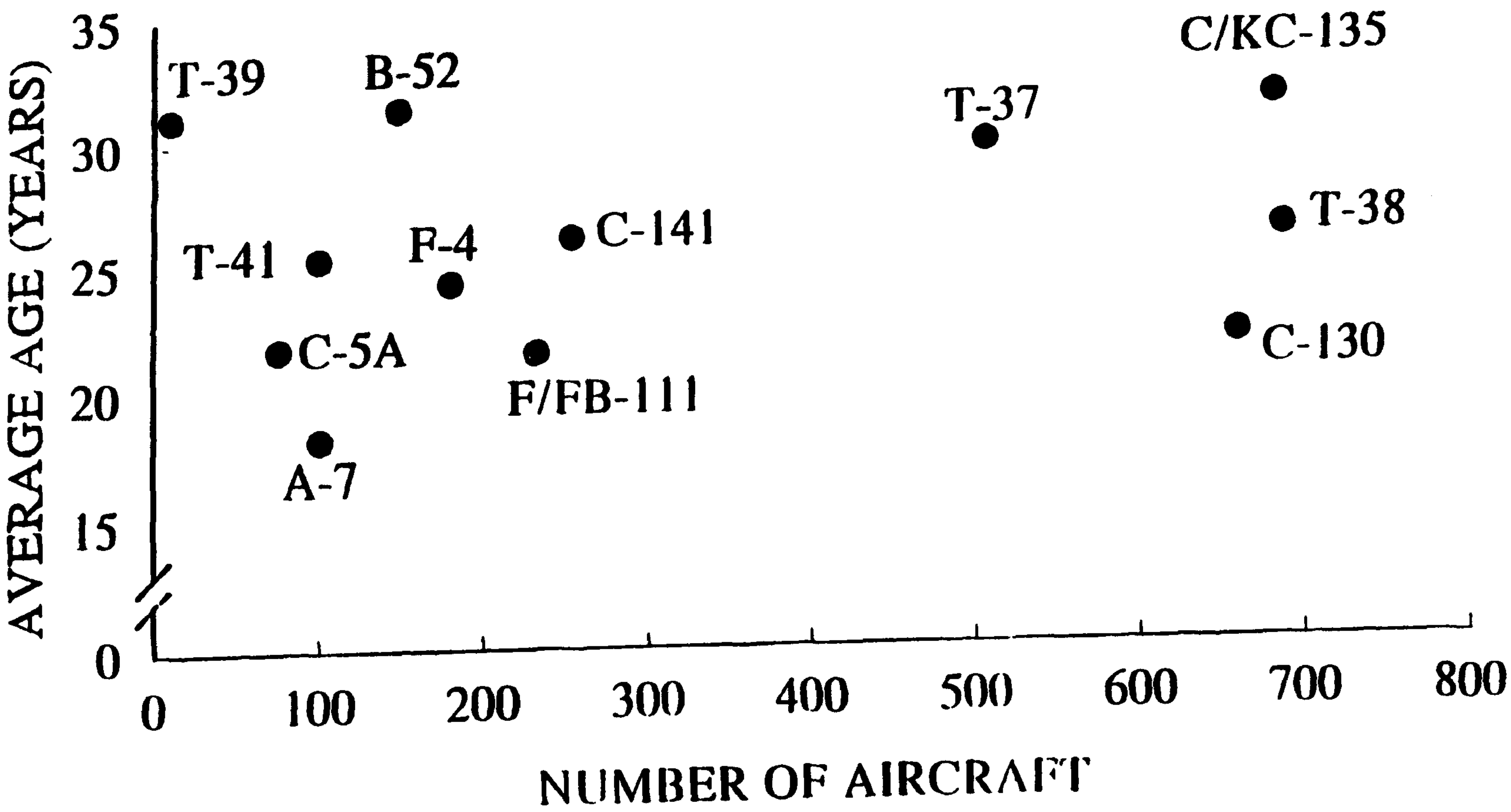
A substantial number of military (as well as commercial) aircraft have been in use for decades, and many have exceeded their originally prescribed lifetimes.

WORKSHOP OBJECTIVE

To survey the technical issues relevant to the life extension of aging airframes and engines of airplanes and helicopters.

AIR FORCE AGING AIRCRAFT

(AS OF 30 SEP 92)



LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

LIFE THREATENING DISEASES

- Fatigue
- Corrosion fatigue

LIFE EXTENSION

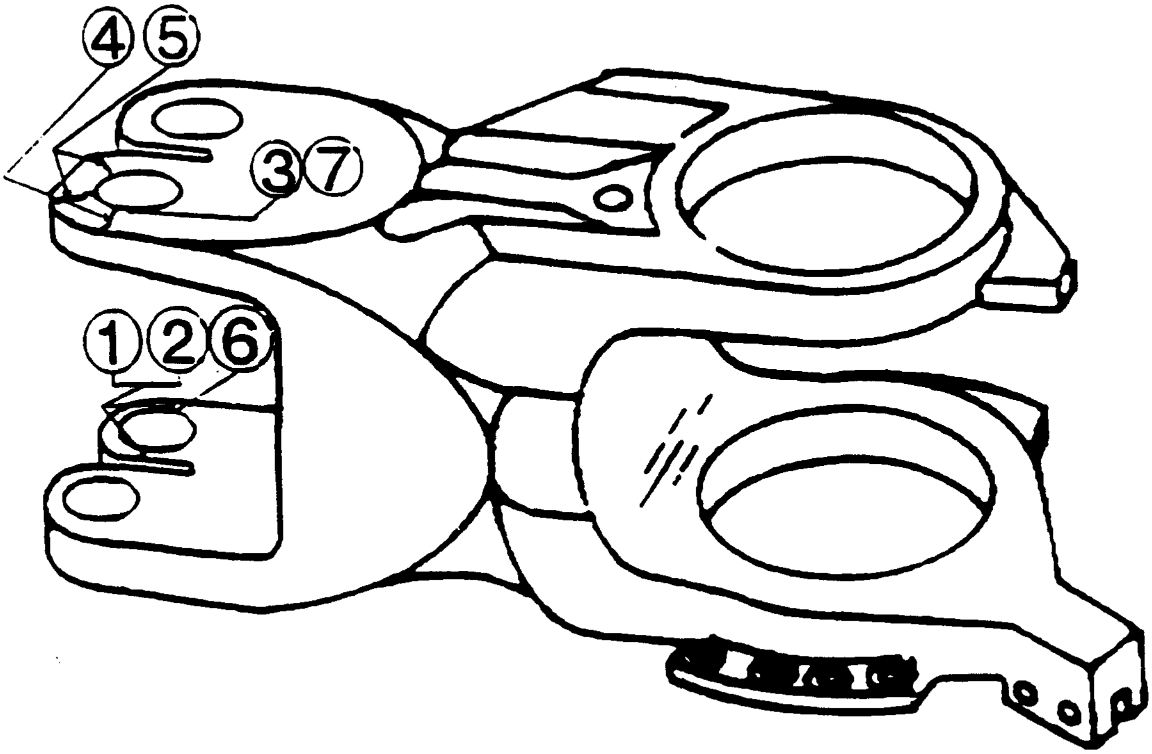
I. Reliably predicted increase in lifetime.

II. Extension of actual longevity: environmental protection; component repair, replacement or reinforcement.

KEY REQUIREMENTS

DAMAGE DIAGNOSIS AND LIFETIME PROGNOSIS

BLADE FITTING



CRACK LOCATIONS

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

TECHNICAL ISSUES

- Fatigue life prognosis.
- Corrosion fatigue life prognosis
- Corrosion protection
- Service history monitoring
- Damage diagnosis
- Active control

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

<u>Fatigue</u>

- Multiple site damage (MSD) studies, residual strength studies, under way (FAA, NASA, AF).
- Needed: reevaluated life estimates ("lifing") based on real-time service history sensing plus retrospective fracture mechanics.

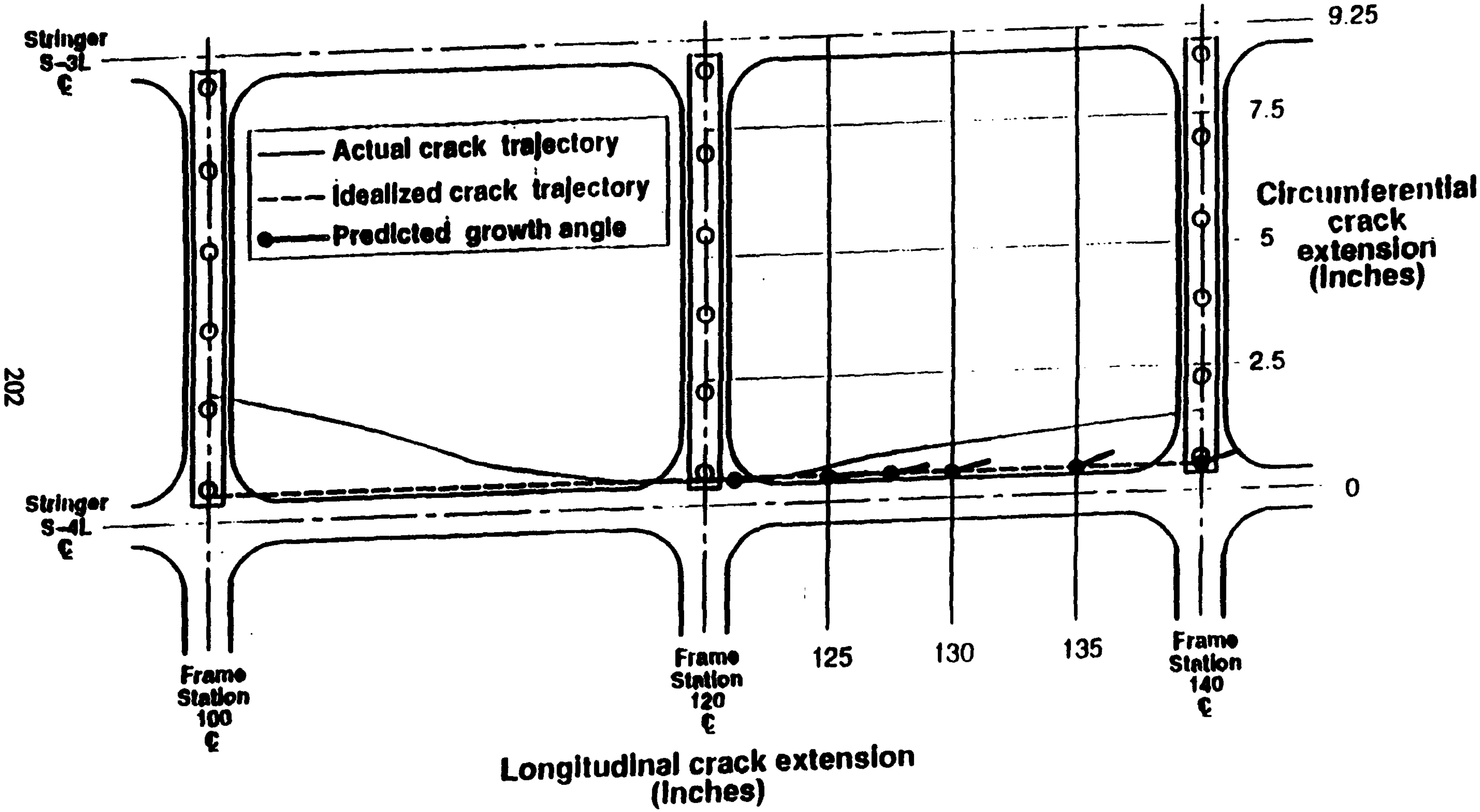
<u>Corrosion fatigue</u>

- Needed: "Paris laws" for corrosion fatigue.
- Continuing need: Basic mechanistic understanding.

<u>Corrosion protection</u>

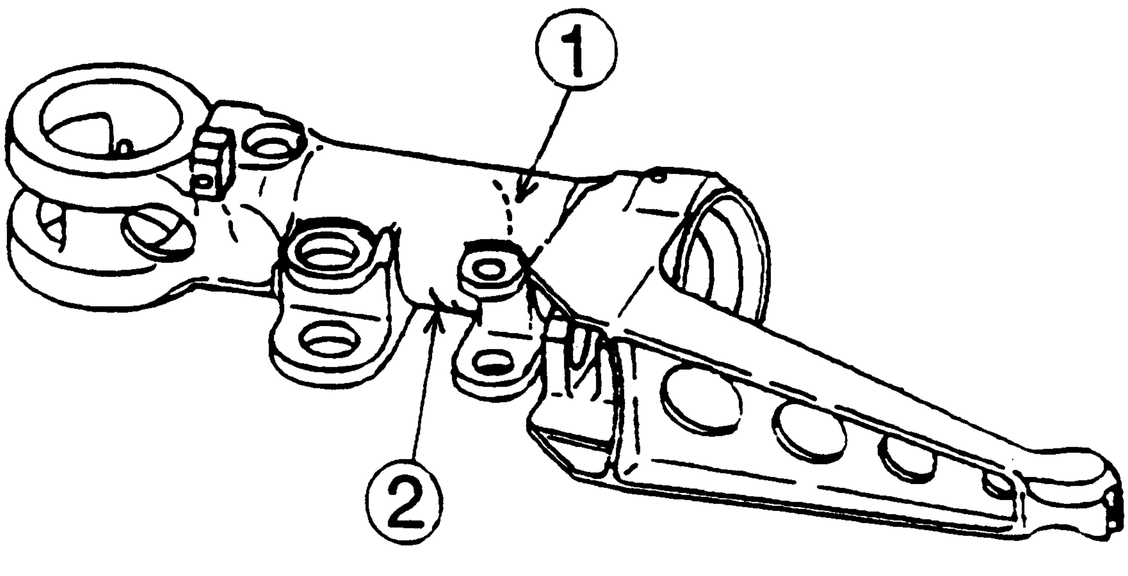
- Electrolytic interaction (e.g. Al,C material plus Ti fastener combos).
- Needed: better protective coatings.

Crack Growth Trajectory For Shear–tied Panel

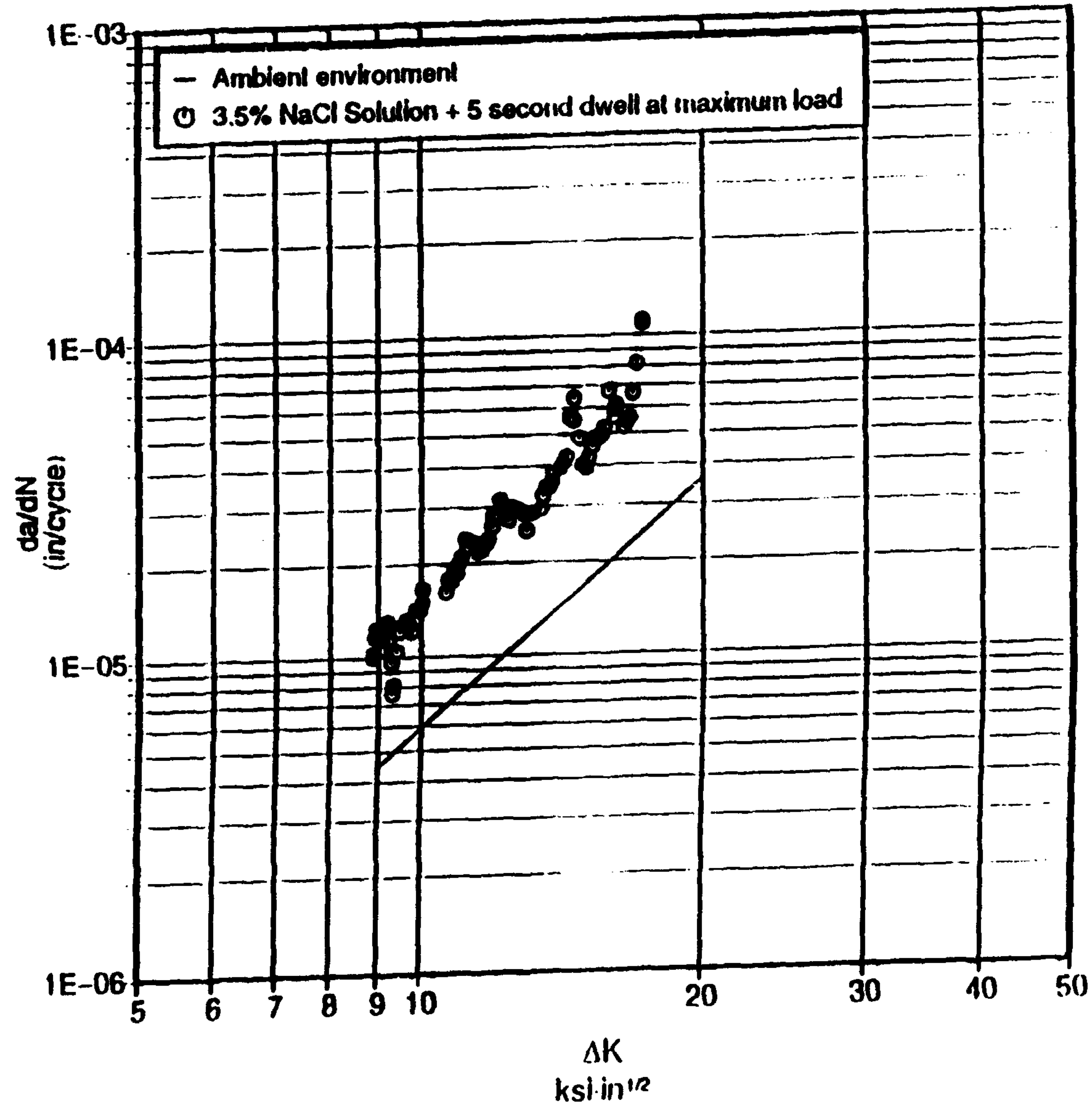


PITCH HOUSING

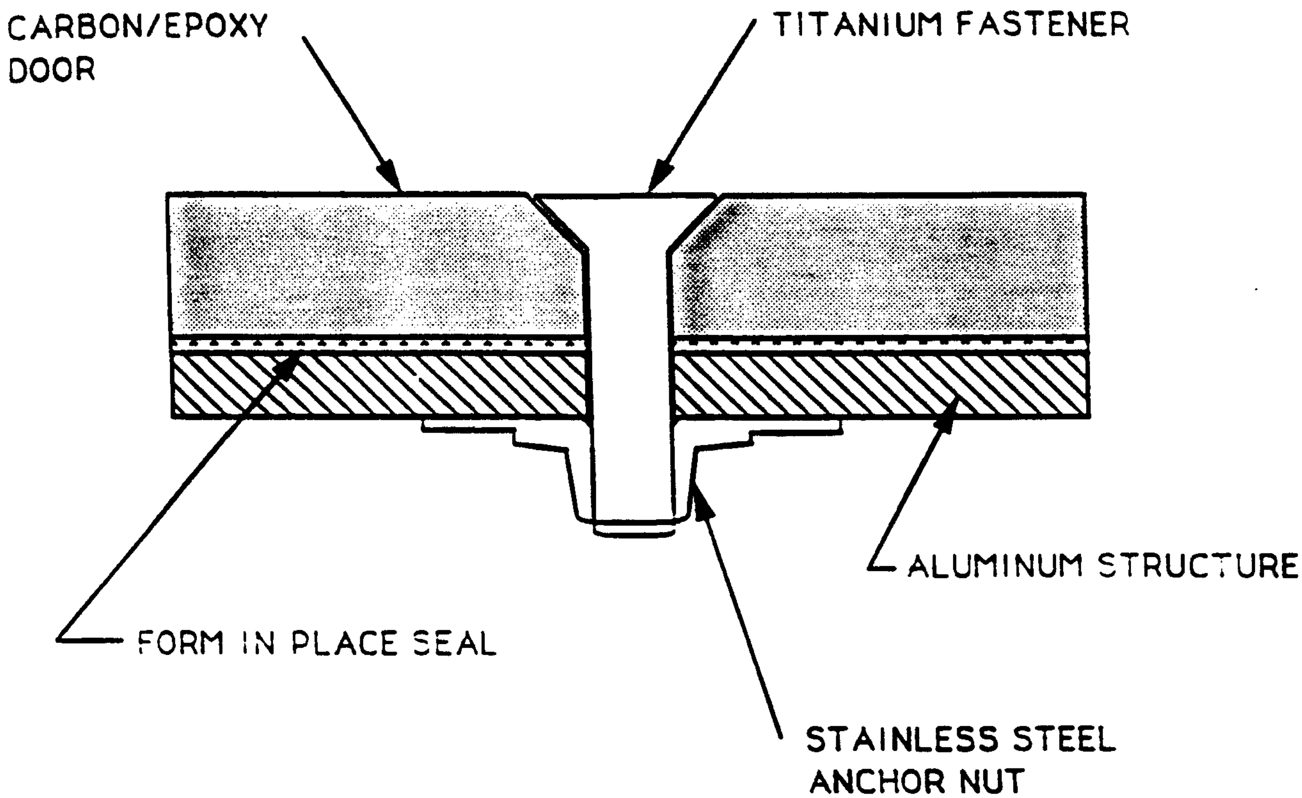
CRACK LOCATIONS



7150-T651



Quality and Integrity Design
Engineering Center (QIDEC)
University of Utah



1. INSPECT/REPAIR FORM IN PLACE SEAL.
2. APPLY CORROSION PREVENTIVE COMPOUND TO FASTENER BORE.
3. START FASTENER IN HOLE.
4. APPLY BEAD OF SEALANT TO FASTENER COUNTERSINK.
5. SET AND TORQUE FASTENER.

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

Service history monitoring

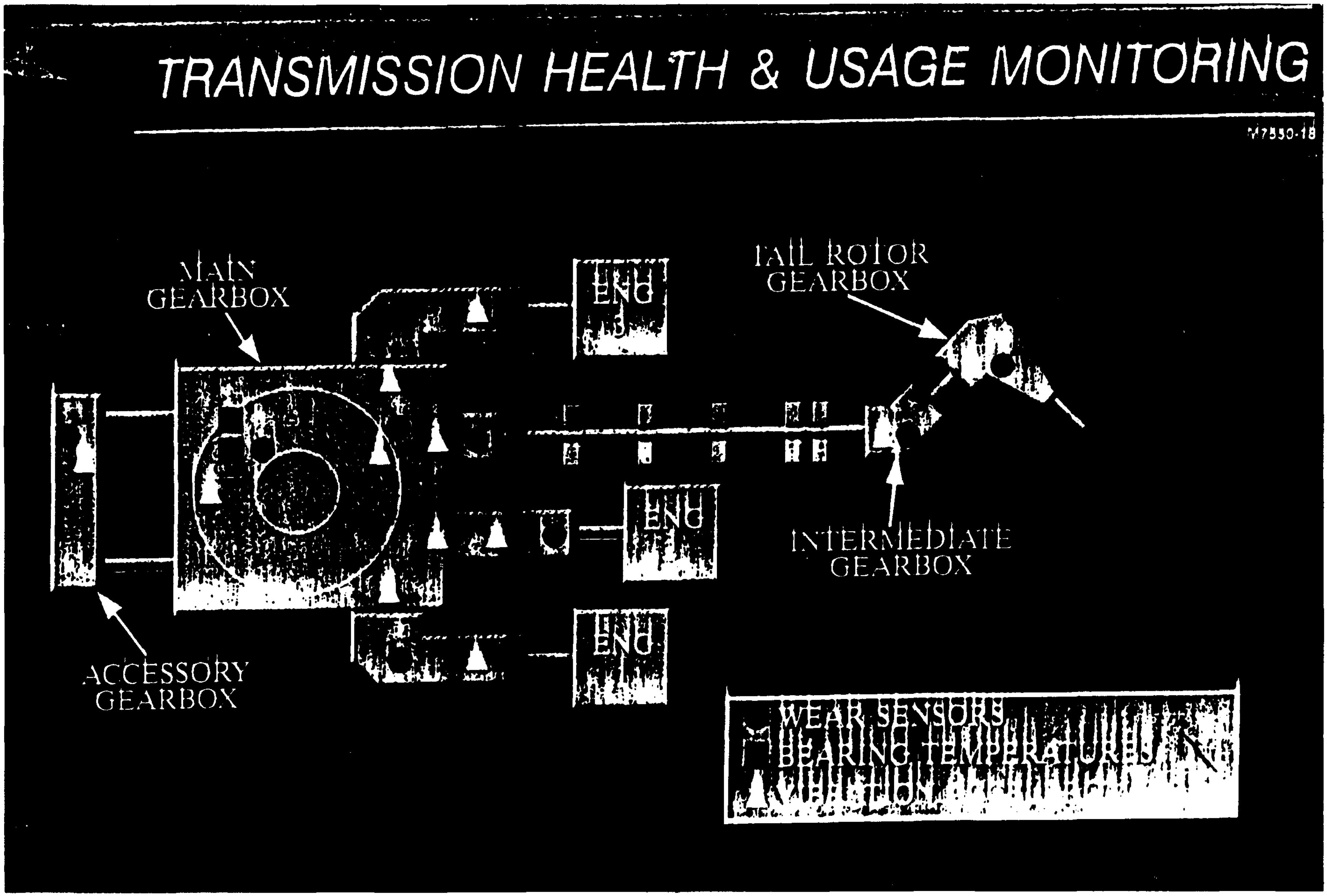
- Sensors (strain, displacement, acceleration).

Damage diagnosis

- Non-destructive crack detection (eddy currents, ultrasonics); probability of detection (POD). Smallest crack?
- Continuous damage sensing; crack-initiation detection? Signal analysis? Feasibility?
- Condition-based maintenance?

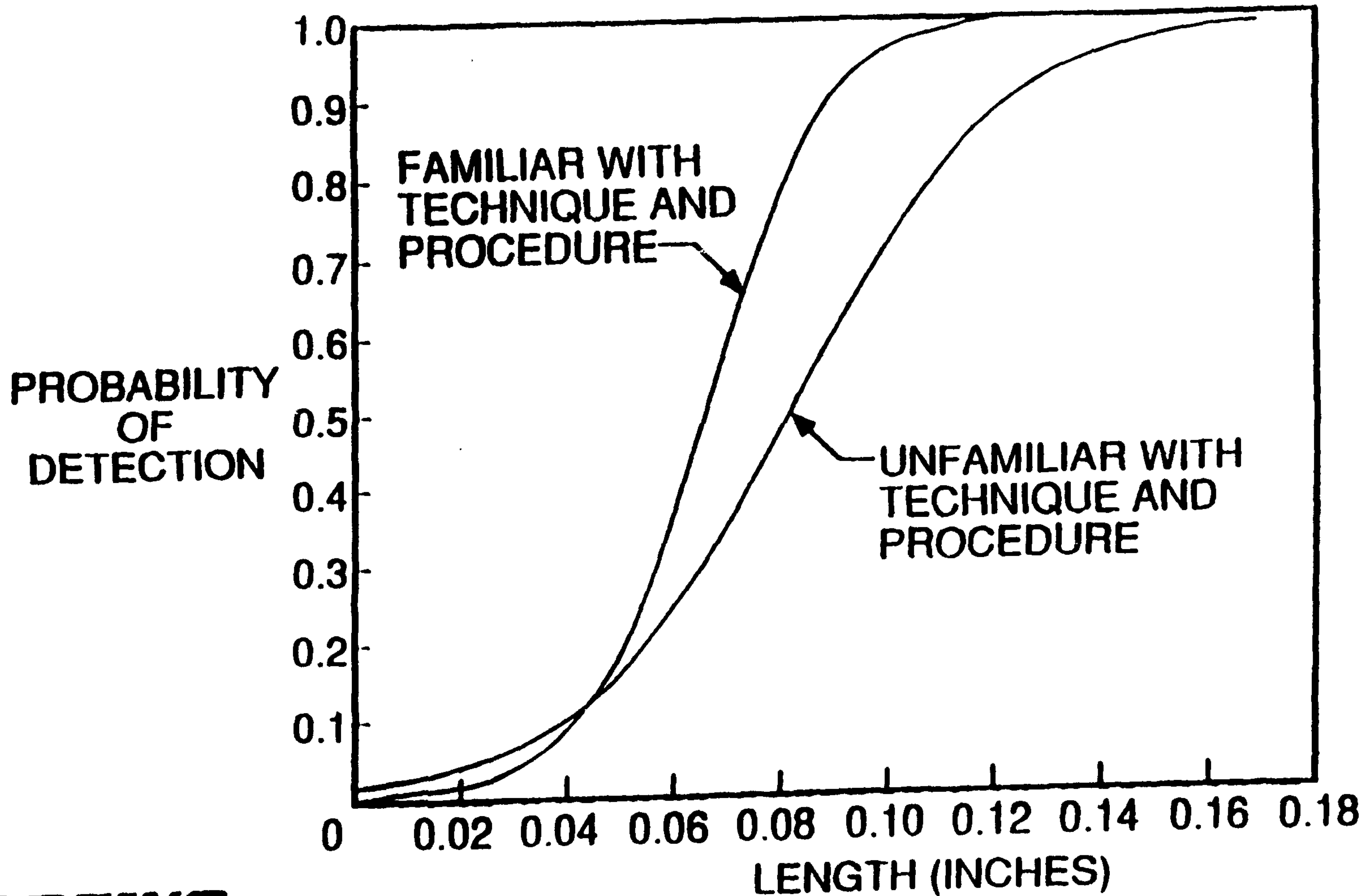
Active control

- Vibration and stress suppression; life-expectancy enhancement.


TRANSMISSION HEALTH & USAGE MONITORING
M7550-18
MAIN GEARBOX
TAIL ROTOR GEARBOX
ENG
ENG
ENG
INTERMEDIATE GEARBOX
ACCESSORY GEARBOX
WEAR SENSORS
BEARING TEMPERATURE

DETECTION PROBABILITY AS A FUNCTION OF CRACK LENGTH

METHOD 3 ROTATING SURFACE PROBE

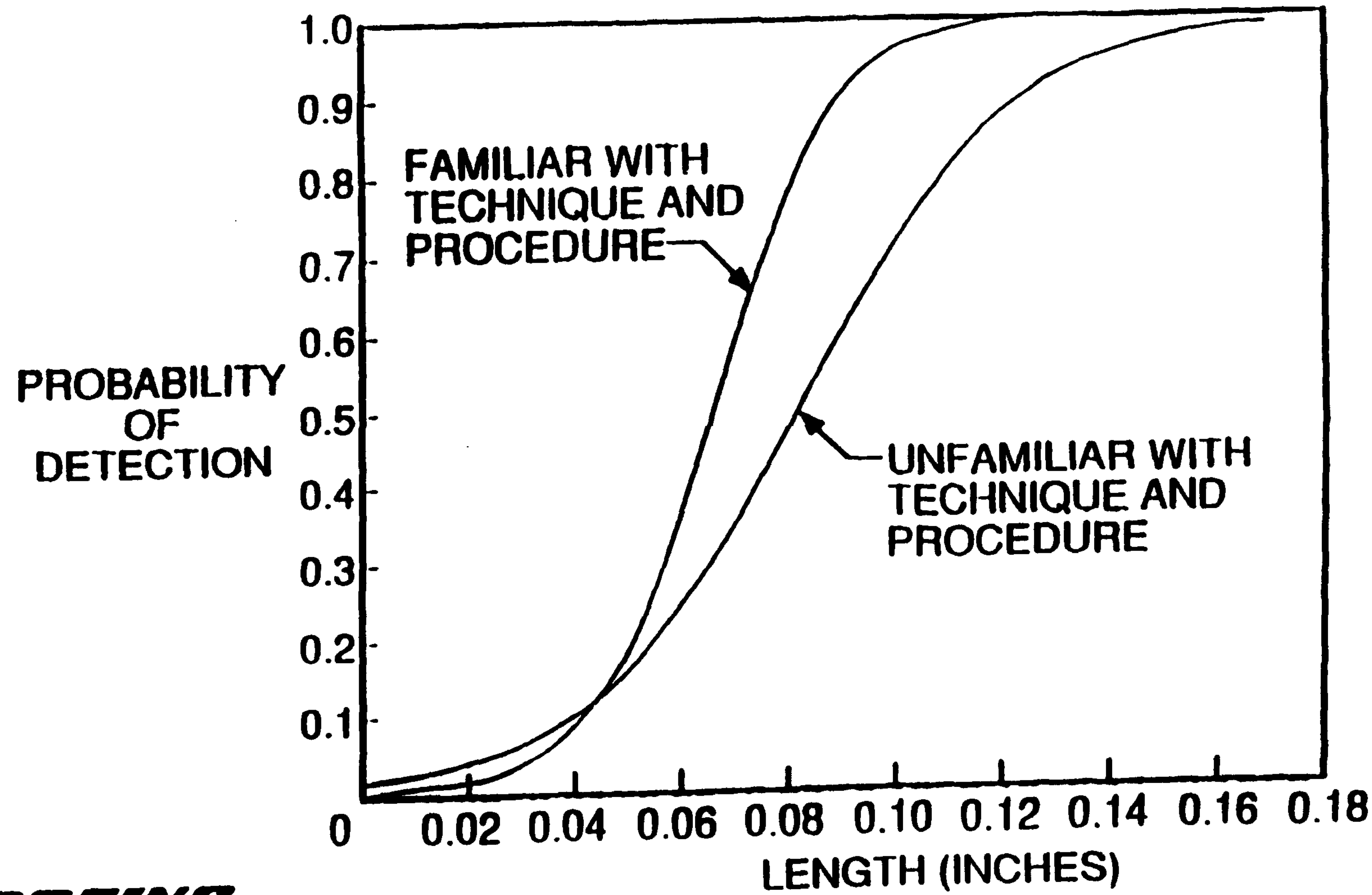


BOEING

CUST. SUP. - HUTCHINSON - 8-24-90
VF-6593

DETECTION PROBABILITY AS A FUNCTION OF CRACK LENGTH

METHOD 3   ROTATING SURFACE PROBE



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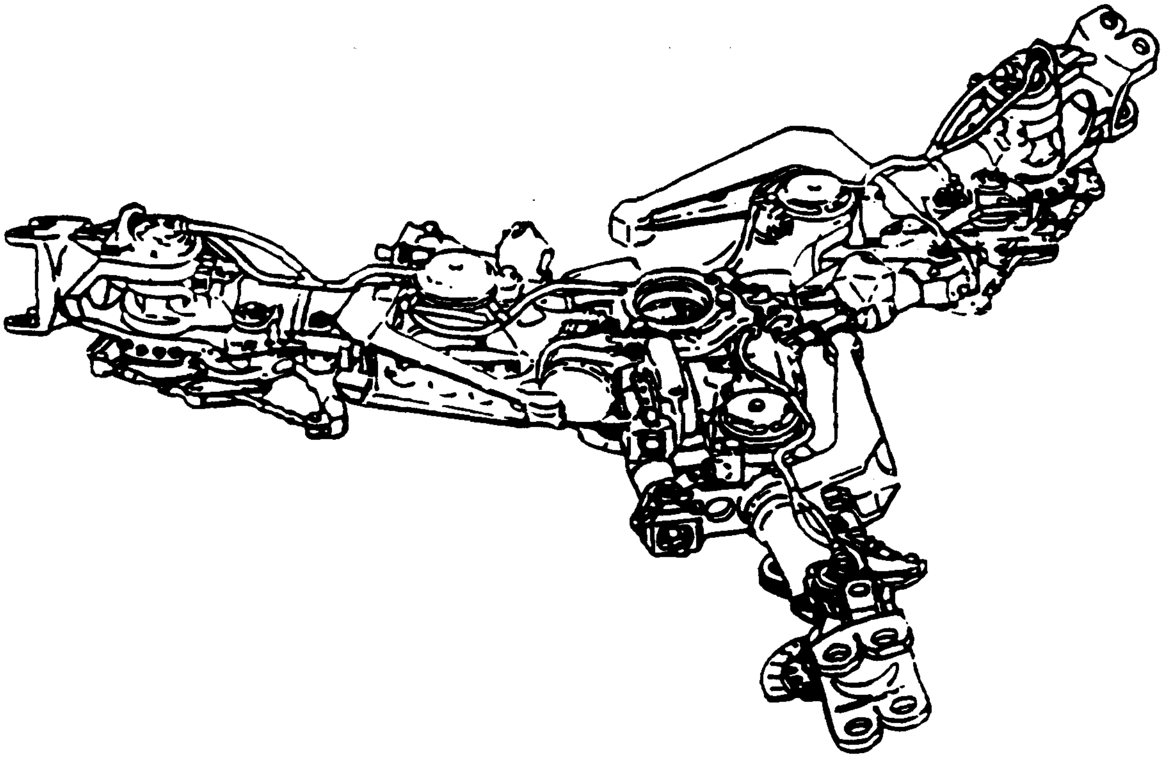
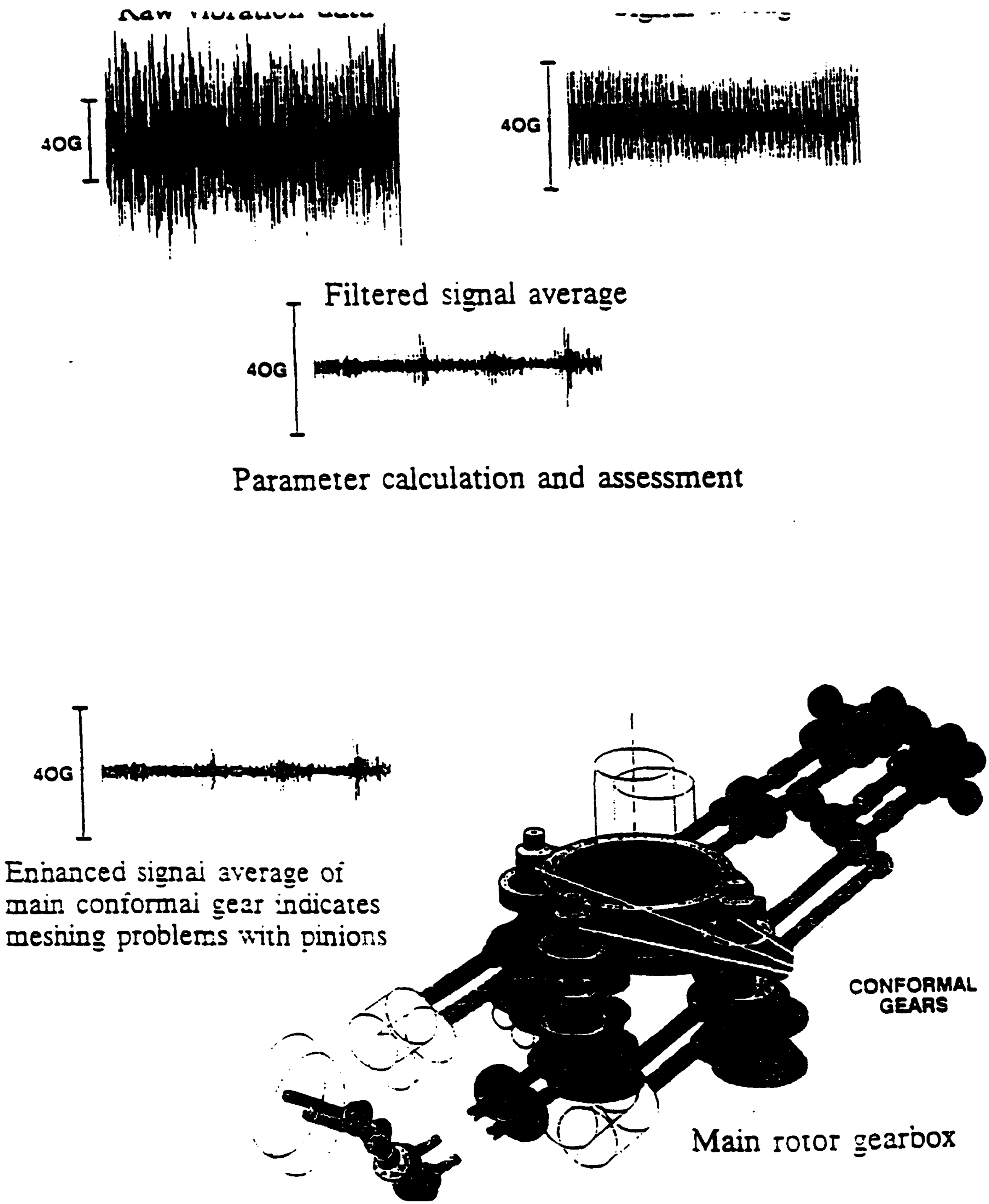
CH -- 46

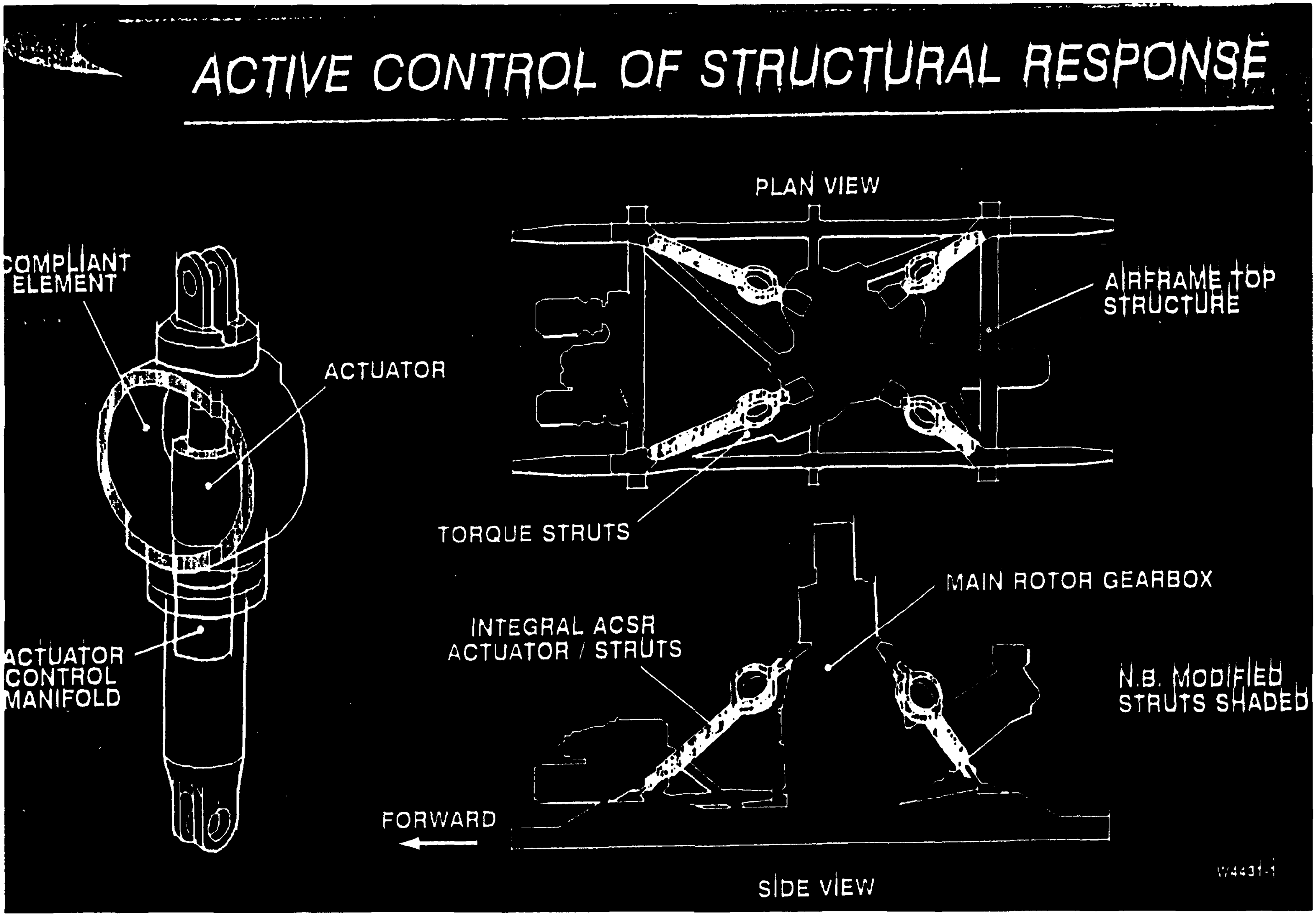
ROTOR HEAD



CURRENTLY 1100 ROTOR HEADS IN INVENTORY
COST --- $ 500.000 EACH



INITIAL DEFECT ASSESSMENT
FIGURE 10



ACTIVE CONTROL OF STRUCTURAL RESPONSE
PLAN VIEW
COMPLIANT ELEMENT
ACTUATOR
AIRFRAME TOP STRUCTURE
TORQUE STRUTS
MAIN ROTOR GEARBOX
INTEGRAL ACSR ACTUATOR / STRUTS
ACTUATOR CONTROL MANIFOLD
N.B. MODIFIED STRUTS SHADED
FORWARD
SIDE VIEW
W4431-1

LIFE EXTENSION OF AGING AIRCRAFT SYSTEMS

CONCLUSION

The discipline of

PROGNOSTICS

integrating continuous on-line sensing with real-time health assessment, fatigue-life updating, and condition-based maintenance is needed to prolong the lives of aging aircraft.

LIFE EXTENSION OF AGING STRUCTURAL SYSTEMS

Workshop Coordinator: John Hutchinson
Morning Session Chairman: Bernard Budiansky

July 20, 1993	
8:00 am	Welcome and Opening Remarks, Bob Crowe (ARPA)
8:15 am	"Life Extension of Commercial and Military Jet Engines", Jim Williams (DSRC/G.E.)
9:00 am	"Managing Maintenance of the F18 as it Ages", Gerald Sturm (Naval Aviation Depot)
	"Corrosion Prevention and Control on the Navy's F18", Mike Albers (Naval Aviation Depot)
10:00 am	Break
10:30 am	"Response to Aging Commercial Airplane Activities at Boeing", Matthew Miller (Boeing)
11:15 am	"Air Force Aging Aircraft Research", Jim Rudd (Wright-Patterson)
12:00 Noon	Lunch
	Afternoon Session Chairman: Tony Evans
1:00 pm	"Current Diagnostic Approaches to Operational Structural Fault Detection", Paul Howard (Howard Consultants)
1:45 pm	"European Approach to Aging Military Aircraft", Dale Milton (ONR, London)
2:30 pm	"Status of Small Crack Detection", Bruce Thompson (Iowa State)
3:15 pm	Discussion
4:30 pm	Adjourn

LIFE EXTENSION OF AGING STRUCTURAL SYSTEMS

July 20, 1993

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PROSPECTS FOR COMPUTATION IN MATERIALS

H. Ehrenreich, A.T. Patera, J.P. Hirth and M.R. Beasley

EXECUTIVE SUMMARY

Workshop Objectives:

To examine the present status of computation in materials science and technology in the context of accelerating the development of modeling and simulation.

Perspective:

A DSRC Workshop on the subject at last years meeting served to define the problems. Important among these problems is the issue of bringing together materials scientists and technologists with the community of numerical analysts and computer scientists. This issue was subsequently addressed in a small off-line workshop which was devoted to discussion of the particular model scientific problem of dislocation modeling. The organizers (H. Ehrenreich, J.P. Hirth and A.T. Patera) prepared extensive background material that was made available to the participants prior to the meeting. (The program and a list of attendees is attached.) Communication between the two communities was easy and relaxed. Its effectiveness is best gauged by at least two examples of collaborations of related problems that ensued subsequently. More importantly, whereas the dislocation problem seemed prohibitively complicated before the workshop, it appeared manageable afterwards. The principal conclusions were summarized at this summer's workshop. (See Scientific and Technological Summary.) While the dislocation problem has both scientific and technological importance, the off-line workshop could equally well have addressed other fundamental questions such as the microscopic description of diffusion in complex systems, martensitic phase transformation, surface scaling reactions such as oxidation, or laser damage. The examination of a single narrowly fo-

cused prototype problem was meant to lay the groundwork for modeling and simulation of processing, design and manufacturing as symbiotic activities of this sort expand.

Finally, it is to be emphasized that the issues being raised here have no obviously simple answers because of the complexity of both materials science and technology and the new computer platforms together with the associated software under current development.

Relevance to DoD

The activities described in this workshop are stimulated by and consistent with the Advanced Materials and Processing (AMPP) and the High Performance Computing and Communications (HPCC) Presidential Initiatives to which ARPA is contributing substantially. The program entitled "Theory, Modeling and Simulation" of AMPP (one of four) is specifically concerned with the issues addressed by this workshop.

The modeling of affordable advanced materials and the simulation of processing steps lead to new materials with more desirable properties at lower development cost. Modeling and simulation is important for the entire range of materials and devices from practically important semiconductor nanostructures to structural materials, and length scales including the atomic, microstructural and continuum. As such, modeling and simulation is basic to both DoD as well as civilian technology.

Scientific and Technological Summary

The session began with an introduction by Jim Crowley, who emphasized ARPA s interest in: (1) a range of materials computations, from atomistic calculations to macroscale process simulations; (2) simulation technology; and (3) the transfer of simulation technology and the resulting benefits to industry. These interests are motivated by the theory/modeling/simulation component of the AAMPP initiative.

The second speaker, Henry Ehrenreich, reviewed the off-line DSRC workshop on Computation of Disclocations held in Washington in May. From the technical side, this meeting (and the preparatory work) iden ti fied several key problems in dislocation theory that could gainfully exploit the cost and speed advantages of parallel computation (see attached), and suggested collaborative mechanisms—between computational and materials scientists—for achieving these ends. Ehrenreich stressed the need for a new computational

physical scientist—either an individual or a group—who uses physically well characterized models and appropriate algorithms to obtain computational results that are physically insightful and/or predictive. He stressed the range of potentially interesting numerical investigations—from simple and exploratory to complex and detailed, from microscopic to macroscopic—and the need for careful attention to physical ingredients and inputs and outputs. A graduate student master/apprentice paradigm for bringing parallel processing expertise into the materials community was proposed.

The third speaker, Paul Messina, presented an overview of Caltech parallel activities centered on the Intel Delta machine. Messina motivated the need for parallel computing and described several examples of successful implementations, from mantle dynamics and fluid flow to galaxy evolution and image processing. He also stressed the pressing need for better parallel I/O, software, and debugging aids. Messina indicated that whereas better, more automatic compilers are certainly important, equally important are robust implementations of current tools. Messina demonstrated for a helioseismological example that parallel computers can serve equally well for both simulation and experimental data analysis. The need for "galactic" geographically distributed computing *environments*, replete with a range of processing servers, workstations, fileservers, and communication infrastructure was emphasized.

The fourth speaker, Anthony Patera, described the motivation for parallel processing in terms of cost and speed. His tutorial on parallel implementation supported a cost benefit analysis for the viability of parallel processing. Two examples of parallel computation were presented, the first the optimization of eddy promoter forced convection heat transfer, the second the calculation of effective properties of random media. Patera stressed that parallel computation is but one part of the study of physical systems; one must also consider physical relevance (validation with respect to experiment), and design relevance (the construction and validation of simplified models for use in engineering design and optimization). Patera demonstrated that even relatively simple problems can exhibit a range of length scales that preclude a purely numerical approach, and proposed that more systematic procedures for the fusion of analytical, experimental, and numerical techniques are required.

A. R. Williams spoke next, beginning with a summary of computational and experimental results for magnetic materials. Williams emphasized the need

for a hierarchy of models involving different length scales, and used the magnetic material calculations as an example of validation. Williams concurred that there were both expensive (uniprocessor supercomputer) and inexpensive (new generation workstations and multiprocessor supercomputer) MFLOPS, and proposed that the most effective approach to parallel computation was a cluster of dual use (e.g., graphics and mail *and* simulation) workstations tightly coupled in a centralized location. Williams suggested that this approach has utilization, technology, and economic advantages that would prove attractive to industry. More generally, he argued that if parallelism is to succeed, industry, and independent software vendors like BIOSYM, must take up the effort. Williams said that parallelism at present only offers faster turnaround, which is not critical to industry. This point was not universally accepted, nor was the concept of centralized and tightly bound, as opposed to distributed and loosely bound or "galactic" work station clusters.

Anders Carlsson addressed the ranges of models and length scales encountered in materials property calculations. He presented examples of *"abinitio"* interatomic force-level, and macroscale simulations that illustrate the range of associated models. In several of his examples, Carlsson aims to predict trends, and even quantitative behavior, at the macroscale by considering microscale quantities "responsible" for, or correlated with, macroscopic behavior. For example, simulations of the crystalline structure of Al_3T for various transition elements T and trace elements (e.g., iron) suggest which metals T might lead to more ductile materials. Similarly, several disclocation problems were proposed related to discussions held at the offline May workshop. Finally, Carlsson described certain applications of parallel processing to parametric studies of many-component alloys.

The next speaker, William Goddard III, described a range of models involving length scales ranging from the quantum mechanical to those appropriate for process control. The talk focussed on a number of large moleculardynamics parallel simulations of different material properties and behavior. The calculations were based, physically, on various force laws and dynamical equations, and numerically, on variations of the Greengard-Rohklin multipole-Taylor series fast many-body-problem algorithm. Goddard described results for a variety of physical problems, including the calculation of surface tension and contact angles for several multicomponent systems. Goddard indicated that the necessary calculations now possible can only be achieved

with parallel machines. His development strategy comprises several steps, starting with implementation of the parallel code on a serial machine, followed by a KSR parallel machine with automatic compilation facilities, and lastly a large message-passing machine (the Intel Delta). Goddard has numerous interactions with industry which might serve as a paradigm for introducing parallel computation by means of collaboration/consultation.

David Srolovitz emphasized the need for workstation-resident design tools that permit engineers to perform what-if experiments. He stressed that these tools must be reliable, but must contain sufficient input information and model simplifications to permit rapid turnaround. As regards ultimate parallel implementations, Srolovitz proposed the workstation cluster as an advantageous, technologically and economically incremental approach, and suggested that trivial parallelism (e.g., with respect to input parameters) is often a viable strategy. Particular physical examples included the calculation of free energies for the construction of phase diagrams and computation of properties such as the effect of surfaces on composition, and computational strategies for extracting more information (e.g., temperature dependence) from a single calculation.

David Ferry spoke about techniques for modeling ultrasmall quantum devices. Ferry indicated that parallelism was, at present, not a leading order concern. He described a range of different models of increasing complexity, from semiclassical moment equations, the density matrix, and the Wigner distribution function, through realtime Greens functions. Sophisticated quantum simulation techniques will become increasingly important as devices become smaller and quantum effects more important.

Tony Evans informally discussed the general problem of transferring materials computing to industry, and described a general framework for understanding the materials, process, and performance interactions. Evans cited the need for good cost models, and for incorporating viewpoints from other disciplines (e.g., dimensional analysis from fluid dynamics). Evans is involved in a continuing academic-industry dialogue, with the next convening of the group scheduled for M.I.T. in the fall.

Conclusions and Observations

Advances in modeling and simulation relevant to materials science and technology depend on (1) the evolution of computing hardware and software, (2) the framework governing the development and application of science and

engineering, and (3) the advance of a relatively recent discipline to be termed here "computational physical science", which complements experimental and theoretical physical science.

The attached view graph entitled "Computer Evolution" describes the current and future computational landscape. For some particular calculation, typical workstations are roughly 5-10 times slower than current uniprocessor supercomputers. Distributed-memory parallel processing permits migration into the favorable "northwest" quadrant: by virtue of being based upon workstation (commodity) technology, distributed-memory multiprocessors are considerably less expensive than uniprocessor supercomputers; by virtue of aggregating many microprocessors, multiprocessor supercomputers are much faster than a single workstation. "Trivial" parallelism (e.g., parameter-based distribution procedures), viable for small problems in which the memory on each processor is sufficient for the entire calculation, achieves speedup of P, the number of processors, whereas "nontrivial" parallelism (e.g., particle/gridbased distribution procedures), appropriate for large problems, achieves lower speedup because of interprocessor communication and increased computation cost in proportion to the parallel efficiency.

In the future, if the past decade is any indication, the computation time for commodity microprocessor technology computers will decrease by roughly 50, and the computation cost will decrease by roughly 500 (a factor of 50 from the increase in speed, and hence decrease in time used, and a factor of 10 from decrease in machine purchase cost). In contrast, uniprocessor supercomputer technology appears largely saturated, with relatively small increases in speed typically accompanied by cost increases. Computation cost reflects direct computer charges (depreciation, lease, or fee); computation time, *if* equated to turnaround time, affects creativity, productivity, and timeliness. Note that any complete cost-benefit analysis for parallel computing must also include the development time and cost required to effect parallel implementations.

The present platforms appear to be adequate for many present day materials science problems. However, problems such as dislocation core-core interactions, or climbing dislocations having kinks, require an explicitly three-dimensional representation and a correspondingly large number (10^6–10^8) of particles. Advanced platforms, capable of parallel computation will be necessary for such applications.

The framework governing the development of science and engineering

may be characterized by technical activities, which include experiment (M_{00}), complex modeling (M_0), and the construction of simple models useful for predicting advance materials with improved properties (M). This kind of partitioning is also useful in engineering design if M_{00} is associated with the characterized physical system, with detailed simulation, and M with the simplified model to be used for processing and design. M may be regarded to be validated by M_0

This framework is illustrated in the appended viewgraph entitled "Scientific Framework" . For specificity, it is convenient to think of transition metals and their alloys, one of the principal building blocks of modern materials technology. "Early Experiments" is to be associated with the measurements of, say, the electrical and magnetic properties. "Phenomenological Theory" of early models include Stoner Theory for ferromagnetism, tight-binding based calculations of the d band structure, the band calculations of the Slater group and Fermi surface experiments showing d electrons to be itinerant. These developments led to LDA based first principle calculations of the electronic structure and a few physical properties like the cohesive energy, status constant, bulk moduli and magnetic moments. (See A.R. Williamss presentation.) Despite their sophistication, these calculations are based on models for describing electronic interactions and certain uncontrolled approximations. The validation of these approximations rests on their empirical success for a variety of materials. The "Simplified Models" , which are useful in predicting trends and pin-pointing alloys and compositions having particularly useful properties, utilize empirical interatomic force laws or simplified band structures to obtain phase diagrams and surface properties. (D. Srolovitz s presentation contains examples.) After this, the spiral shown in the viewgraph evolve into the next loop in which more practical transition metals and alloys containing defects are addressed. The next cycle, denoted by M'_{00}, M' *and* M'_0, mimic the first. The presence of defects such as impurities, dislocations, grain boundaries and cracks makes the complex calculations denoted by M'_0 far more complex, and *without doubt* necessitates the use of massively parallel computations. The calculations of dislocation interactions and kinks considered during the May Workshop are simple by comparison!

These calculations may validate already existing simpler models, M, or others that remain to be invented—models that will have real utility in materials design. The next loop in the spiral will, without a doubt, address the all-

important dynamics questions encountered for example in diffusion, crack propagation and fracture. The present understanding of these complex processes on a microscopic basis is very limited indeed.

The contents of the two viewgraphs just discussed may well represent a programmatic outline of activities in the modeling and simulation area.

The remaining missing ingredient is the present scarcity of computational physical scientists described in Ehrenreichs summary of the May Workshop. The viewgraph entitled "The Kinds of Physical Scientists" defines the attributes of this scientist (in reality, a small collaborative group at least at the outset). The computational ingredients of this new science are outlined in the viewgraph under that title.

We summarize this discussion by emphasizing several items. First, the recognition of a range of length scales, associated models, and necessary computational platforms, and the need for validation of each level of model in terms of experiment and more complex models in the hierarchy; second, the need for better experimental data, perhaps the identification of key experiments, and, in general, better organization of existing experimental and numerical results and methodology; third, the importance of working with independent software vendors to ensure that computational techniques for materials science—including but certainly not focused on parallel implementations—make their way into industrial practice.

A program to stimulate modeling and simulation development must therefore include the following ingredients: The computational ability of the community must be developed. There may be merit in a fellowship or other program fostering a master-apprentice relationship, in which graduate students or other scientists associated with a materials group working on a particular problem affiliate themselves with a group devoted to advanced computing platform exploitation and algorithm development in order to solve that problem. Advanced computing platforms together with the necessary software should be made generally available to the materials science and technology community within the next three years in order that the evolution of the spiral shown in the Scientific Framework viewgraph not suffer undue delay. The necessity for calculations at all levels of sophistication must be recognized. The fact that calculations emphasizing trends in related materials rather than numerical accuracy can be predictive is also important in guiding the path to new materials in more cost-effective ways than approaches based entirely on Edisonian invention.

PROSPECTS FOR COMPUTATION IN MATERIALS

H. Ehrenreich, A. T. Patera, J. P. Hirth
and M. R. Beasley

Objective

- Accelerate development of modeling and simulation in materials science and technology.

DoD Relevance

- Modeling affordable advanced materials and processing leads to new materials with more desirable properties
- Modeling and simulation spans practically important semiconductor nanostructures through structural materials, and length scales ranging over atomic, microstructural and continuum.
- Workshop stimulated by and consistent with AMPP and HPCC initiatives.

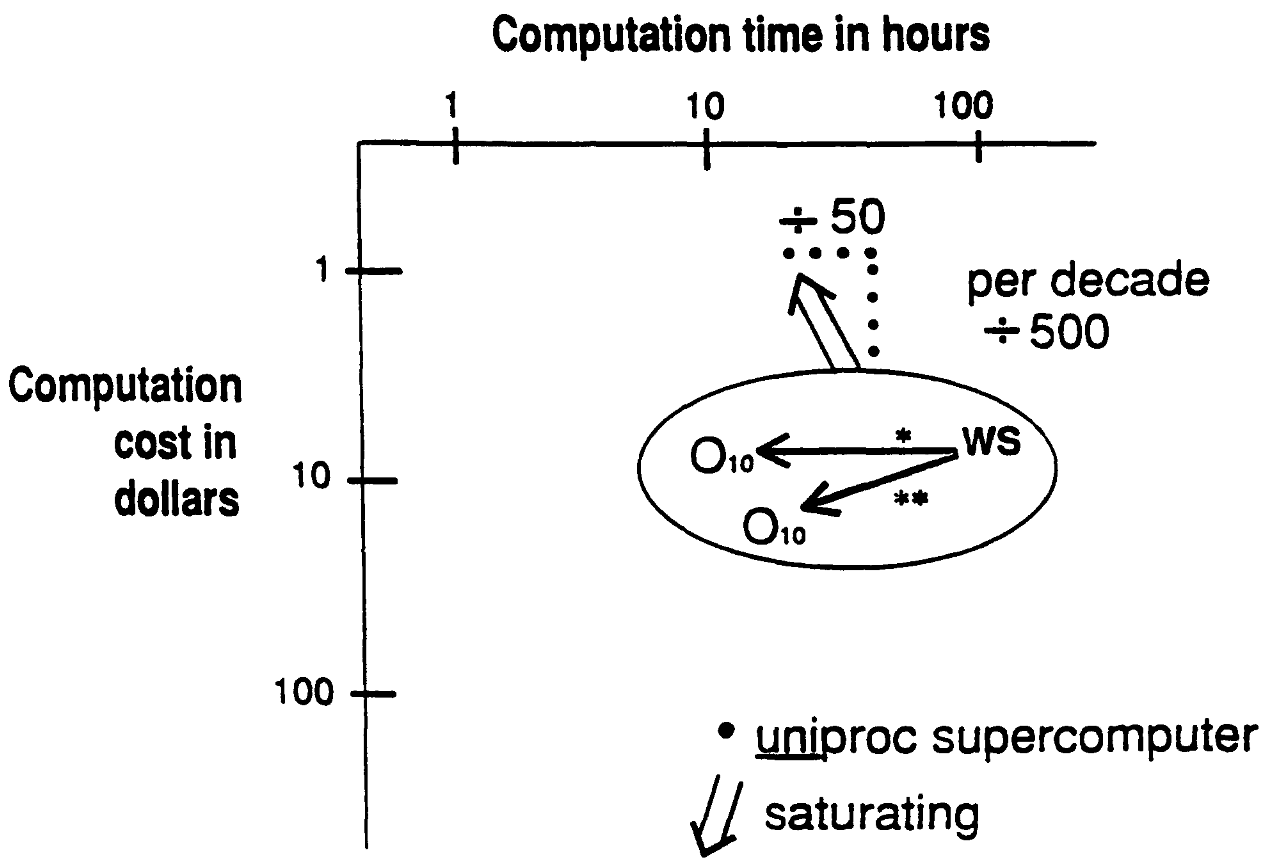
Scientific and Technological Issues

Rapid modeling and simulation advances depend on

- Computer evolution
- Scientific and technological needs
- A new kind of scientist:

Computational Physical Scientist

Computer Evolution

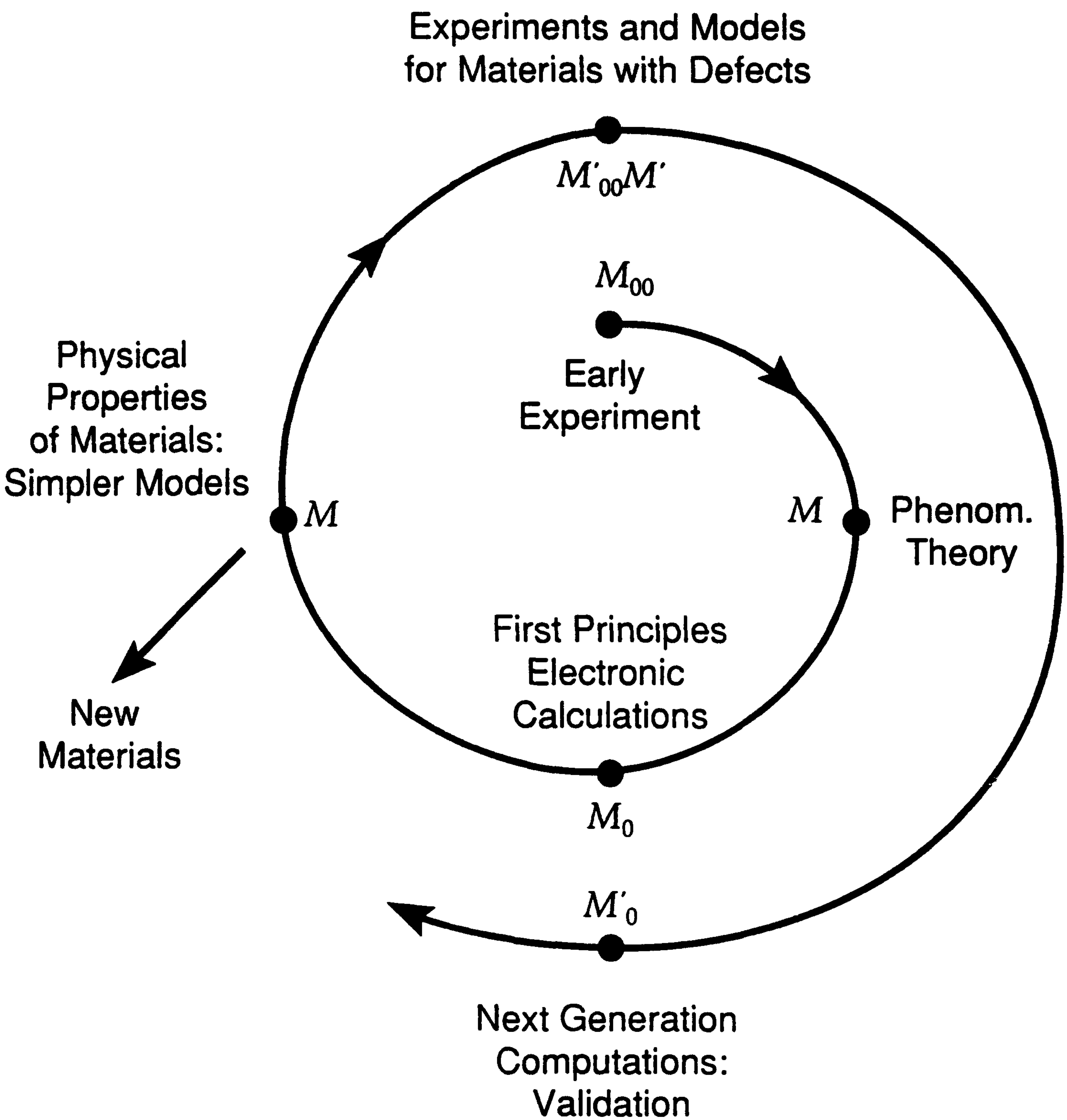


O10 **10-proc distributed-memory parallel machine, cluster, ...**

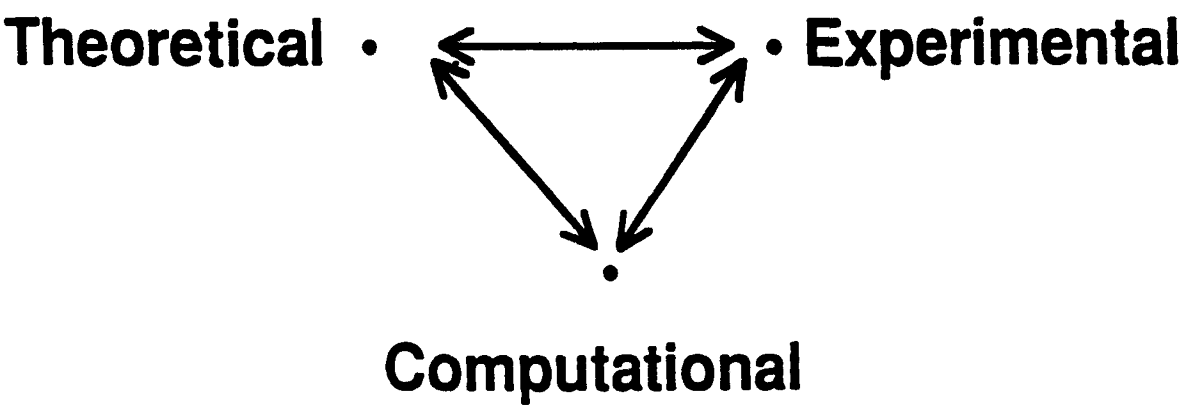
* **trivial parallelism**

** **nontrivial parallelism**

Scientific Framework



The Kinds of Physical Scientists



"Computational Physical Scientist"

Interactive physical science/numerical analysis ***partners,*** *who use physically well characterized models and appropriate algorithms to obtain computational results that are physically insightful and/or predictive.*

Computational Ingredients

- **Wide Range of Physical Models**

  — Simple, exploratory:
  New physical effects
  ("Ising Model")

  — Complex, detailed:
  Realistic Simulations
  (Ion Implantation)

  — Macroscopic → Microscopic
  (Continuum → Quantum mechanical)

- **Physical Ingredients**

  — Different Length Scales

  — Many Particle Interactions
  (Local Density Approximation)

  — Force Laws
  (Science or Engineering Motivated)

  — Empirical Macroscopic Relations
  (Constitutive Equations)

- **Assessment of Input/Output**

  — Wide spectrum of uncontrolled approximations: require validation methodology

  — Comparison with experiment and results of simple models

  — Exploration of Force Law/Physical Property Relationships

Conclusions and Observations

Ways of stimulating modeling and simulation:

- Develop computational capability of community:
  - Master/Apprentice Relationship
  - Fellowships possibly associated with Technology Reinvestment Program
- Make advanced computing platforms and associated algorithms generally available to material scientists.

  Time scale: ~ 3 years
- Recognize that calculation of trends in homologous materials can be predictive, guiding the path to new materials cost effectively (compared to an Edisonian approach)

PROSPECTS FOR COMPUTATION IN MATERIALS

Workshop Organizer: Henry Ehrenreich
Workshop Organizer: Anthony T. Patera

July 21, 1993

8:00 am	ARPA Perspective, J. M. Crowley (ARPA)Introductory Comments, H. Ehrenreich (DSRC/Harvard University)
8:30 am	"Parallel Computing: Progress and Prospects. (The View from the Trenches)", P. Messina (Caltech)
9:15 am	"A Parallel Tutorial", A. T. Patera (DSRC/MIT)
10:00 am	Break
10:30 am	"Computers and Materials Design", A. R. Williams (IBM, Yorktown Heights)
11:15 am	"Strategies for Computer Aided Materials Design", A. Carlsson (Washington University)
12:00 Noon	Lunch
1:00 pm	"New Methods for Atomistic Simulation for Large Systems (Million atoms per unit cell)", W. A. Goddard (Caltech)
1:45 pm	"Perspectives for Efficient Atomistic Simulations of Solids and Their Defects", D. Srolovitz (DSRC/University of Michigan)
2:30 pm	"Modeling of Quantum Transport in Semiconductor Devices", D. K. Ferry (DSRC/Arizona State University)
3:15 pm	Discussion
4:00 pm	Adjourn

PROSPECTS FOR COMPUTATIONS IN MATERIALS

July 21, 1993

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APPENDIX

MATERIALS/COMPUTATION WORKSHOP
DISLOCATION DYNAMICS

H. Ehrenreich, J. P. Hirth, A. T. Patera
(Organizers)

May 24-25, 1993

SPC, Arlington, VA

Materials/Computation Workshop:
Dislocation Dynamics
May 24-25, 1993
Organizers: Henry Ehrenreich, John P. Hirth, Anthony T. Patera

Participants:

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Materials/ Computation Workshop: Dislocation Dynamics

Preliminary Program

Monday, May 24

10:30 am — ARPA Perspective: **Crowley**

Statement of Dislocation Problem: **Hirth** (1 hour)

Numerical Execution of a Related Problem; **Hoagland** (30 minutes)

Lunch

1:30 pm — Case Study: Parallel Simulation of Viscous Incompressible Flows; **Patera** (45 minutes) (Relevant Computational Kernels)

2:30 — Experiences with Scalable High Performance Computing; **Johnsson** (45 minutes) (CM calculations in solid state, solid mechanics, basic algorithms)

3:30 — Force Laws, Boundary Conditions, Peierls Stress Calculations: **Carlsson** (45 minutes)

4:30 — Dislocation Dynamics, Stacking Fault model of Peierls Barrier, Other Computational Aspects: **Kaxiras** (45 minutes)

5:30 — Discussion Period: e.g. further exploration of dislocation dynamics problem, etc.

6:00 — Adjourn

Tuesday, May 25

8:30 am — Discussion: Conclusions and Recommendations: **Ehrenreich**

Questions to be addressed (plus others raised by workshop participants):

- What is specific physical or engineering question being asked?
- How many particles (degrees of freedom) must be considered to achieve reliable results and what are the key computational kernels?
- How can analytical information be used to reduce the computational degrees of freedom?
- What are computational requirements (architecture, algorithms, codes)?
- How can interactions between materials science/numerical analysis/computer science communities be improved?
- What are the time scales for computer and physical modelling development necessary to solve the dislocation problem?

12:30 — Adjourn

BACKGROUND MATERIAL

Materials/Computation Workshop: Dislocation Dynamics

H. Ehrenreich, J.P. Hirth, A.T. Patera
(Organizers)

May 24-25, 1993
SPC, Arlington, VA

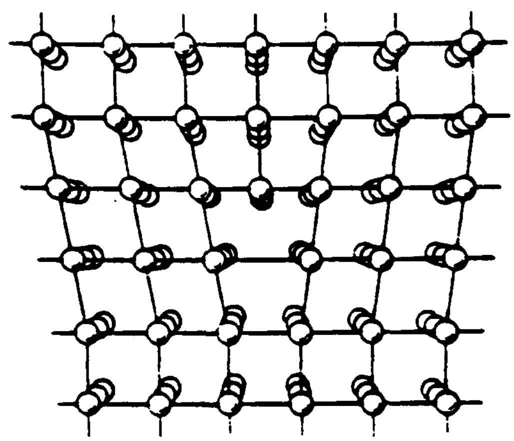


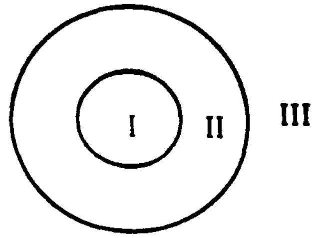
FIGURE 1-4. An edge dislocation in a simple cubic crystal.

Dislocation Simulation

Calculation

1. Compute $u_i^*(x_i)$ **elastic** displacements due to dislocation for all atoms i position x_i, and displace atoms. This is the zeroth order solution of the problem.

2. Divide the space surrounding the dislocation into three cylindrically concentric regions: I, II, III.
Using cylindrical symmetry, assume that slices along z-axis (perpendicular to page) are thin (~ 2-5 layers).



3. Relax I while holding atoms in II & III fixed
   -- Find potential energies E_i in regions I and II:

$$E_i = F_i(\rho_{ij}) + \frac{1}{2}\sum_{i \neq j} \varphi_{ij}(r_{ij})$$

$F_i(\rho_{ij}) =$ non-pair embedding potential: cuts off after 3-4 neighbors

$$\rho_{ij} = \sum_{i \neq j} \rho_j^a(r_{ij})$$

$\rho_j^a(r_{ij}) =$ spherically averaged atomic electron density

$$\varphi_{ij}(r_{ij}) \propto \left[1 - e^{-\alpha(r_{ij} - r_i)}\right]^2 - 1$$

empirical pair potential (Morse form)

   -- Compute force F_i on atom i:

$$F_i = -\nabla E_i$$

   -- Fixed Boundary Conditions: Atoms in II and III fixed, but these atoms exert forces on I.

   -- Relax atoms in I, using Newton's Second Law:

$$\dot{x}_i(t + \delta t / 2) = \dot{x}_i(t - \delta t / 2) + (F_i / m)\delta t$$

$$x_i(t + \delta t) = x_i + \dot{x}(t + \delta t / 2)\delta t$$

   -- Quench kinetic energy periodically to approach minimum energy for static equilibrium.

4. While the displacements in I are determined by microscopic forces, those in II are determined by macroscopic elastic forces. One procedure is to relax II while holding atoms in I (as previously relaxed) and III fixed.
   -- Calculate forces F_i on atoms in II using the relaxed atoms in I and unrelaxed atoms in III.

   -- Convert to f_i, forces per unit length along z

   -- Use linear elastic Green's function to compute the elastic displacements in II:
$$u_i = G_{ij} f_j$$

5. Remove remaining internal strain in system, which remains because of non-linear distortion in I, by iterating, repeating 3 and 4 until equilibrium is obtained.

6. Alternatively, one could relax I, II and III elastically, instead of just region II as suggested in 4 and then iterate by repeating 3 and 4. Both procedures will converge to the same result, but one may be faster than the other.

Notes on Size of Regions I, II and Boundary Conditions

1. Presumably size of I is no smaller than 3-4 nearest neighbors. This is the distance where Hoagland, *et al.*(1) cut off ρ_{ij} and φ_{ij}. Hoagland *et al.* also point out that II becomes less important for larger I. Their largest model contains 2300 atoms having diameter 100Å and 5Å thickness (6 layers). Regions II and III are treated using fixed boundary conditions. There is no self-consistency procedure as that implied by 5. above.

2. Implementing self-consistency is easier if I is chosen as large as Hoagland *et al.* do.

3 Region II should have size no smaller than the cut-off distance.

4. Flexible Boundary Conditions, according to Hoagland, complicate numeric calculations somewhat, but make a smaller region I possible.

5. *How many atoms are necessary for a reliable description?*

Dynamics

Formal physical model remains to be developed.(2) (Some current work will be described by Kaxiras and others.)

References:

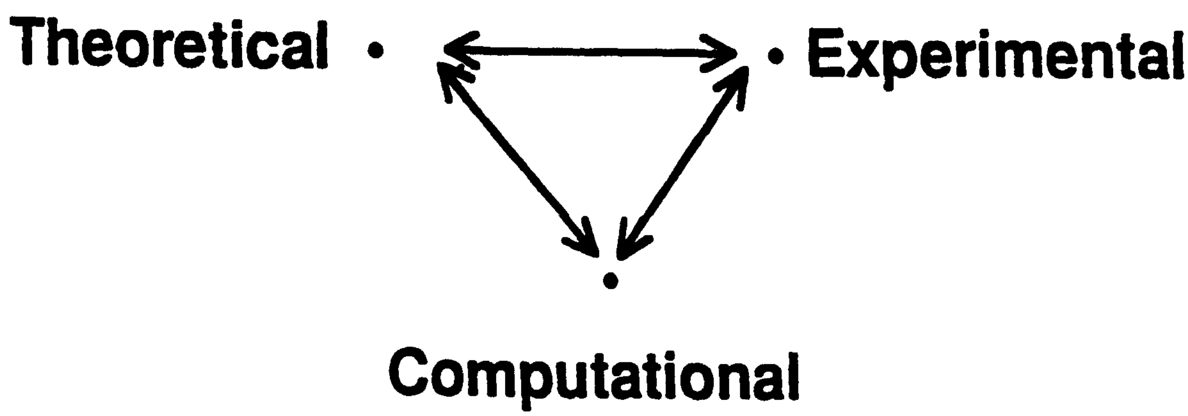
(1) R.G. Hoagland, M.S. Daw, S.M. Foiles and M.I. Baskes, *J. Mat. Res.* 5, 313 (1990).

(2) See J. Lothe and J.P. Hirth, *Phys. Rev.* **115**, 543 (1959).

General Conclusions

MATERIALS/COMPUTATION WORKSHOP DISLOCATION DYNAMICS

The Kinds of Physical Scientists



"Computational Physical Scientist"

*Interactive physical science/numerical analysis **partners,** who use physically well characterized models and appropriate algorithms to obtain computational results that are physically insightful and/or predictive.*

Capabilities

- Numerical Realization of Physical Theories
- Algorithm Development addressing
  - — New Problems
  - — New Computer Architectures

    (e.g., Massively Parallel Computation)
- Effective Use of Existing Algorithms
  - — Creation and Use of Libraries

Computational Ingredients

- **Wide Range of Physical Models**

  — Simple, exploratory:
  New physical effects
  ("Ising Model")

  — Complex, detailed:
  Realistic Simulations
  (Ion Implantation)

  — Macroscopic → Microscopic
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- **Physical Ingredients**

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  (Constitutive Equations)

- **Assessment of Input/Output**

  — Wide spectrum of uncontrolled approximations: require validation methodology

  — Comparison with experiment and results of simple models

  — Exploration of Force Law/Physical Property Relationships

Comments

- Tension between Science and Engineering:

  An opportunity, not an inhibition!

- Computational Sophistication should match:

  — reliability of input data

  — limitations imposed by projection (finite number of particles)

- Conclusions should be understood and articulated as clearly as the best experimental or theoretical physical science.

  They may be equally profound!

The Basic Question

How can Development of Computational Physical Science be accelerated?

— Esteem/Reward Structure for Practitioners

— Master/Apprentice Paradigm for Learning

— Plus??

THERMOPLASTIC MATRIX COMPOSITES

James Economy

EXECUTIVE SUMMARY

Workshop Objective

The intent of this workshop was to assess the current status of the field of Thermoplastic Matrix Composites (TPMC). With the major downsizing of DoD programs including those on polymeric composites it seems very timely to examine recent progress in TPMC and assess the problem areas as well as opportunities that will emerge under the changing ground rules of the future. Toward that end a workshop was organized which included suppliers of thermoplastic resins, both DoD and commercial fabricators of composites and representatives of the funding agencies who have been supporting this field. Of specific interest was the question concerning future R&D in this area and in particular, the need for improved manufacturing processes as well as lower cost fibers and matrices. An attempt was made to address several common misconceptions associated with TPMC, such as poor compressive properties and difficulties in their fabrication. The potential withdrawal from the market by several major resin suppliers primarily as a result of DoD downsizing suggests a requirement for a new strategy to sustain development of this field. The need to define and implement such an approach is especially critical with the potential threat of losing this entire field of endeavor to the Japanese who continue to commit significant R&D resources to the field of composites.

Relevance to DoD

TPMC is a fairly new field which was initiated in the early 1980s primarily with Air Force support. This area should be distinguished from injection moldable composites based on chopped fiber which have been commercially available for over 25 years. For DoD, TPMC may offer several advantages over composites based on thermoset resins. These include potential for improved resistance to impact damage, simplified joining and repair, moisture resistance

and the possibility for automated manufacture. The TPMC's also have a potential for significantly enhanced thermo-oxidative stability as compared to thermosetting matrices which because of the nature of the crosslinking units are intrinsically unstable in air at temperatures of 200°C (even lower during extended use).

Starting in 1987 the Air Force began to support a major development program on TPMC encompassing 1) continued work on advanced materials & processing 2) manufacturing science, technology and advanced development, and 3) supply/repair. A number of component parts have been successfully prepared and evaluated for use on eight different aircraft. Data showing advantages of TPMC over thermosets such as BMI has been generated. A reliable data base now appears to exist for a number of secondary structures in military aircraft. A program is underway to evaluate both TPMC and thermosetting matrix composites (TSMC) for advanced submarines because of their greatly improved damping characteristics. Other government supported programs for TPMC and TSMC include NASA's effort on a subsonic and a high speed civil transport (HSCT) and DOE's proposed five year program on lightweight material for automobiles.

For the future, increasing concern on the part of DoD with respect to recyclability and lifetime extension of thermoset composites may represent important opportunities for TPMC.

Scientific and Technical Summary

In this section discussions are provided on the following four themes:

- Matrix Considerations
- Fiber Considerations
- Component Manufacturing
- Business Strategies

Matrix Considerations*

The advantages of thermoplastic over thermosetting matrices were spelled out during the workshop. These include the possibility of higher impact resistance, higher thermo-oxidative stability, long shelf life, reprocessability, moisture resistance, and low outgassing. Within the field of thermoplastic matrices those that are semicrystalline offer advantages over the

amorphous polymers since they display better solvent resistance and lower moisture absorption. In addition they have a potential for better creep resistance at elevated temperatures compared to the amorphous polymers. The ability of thermoplastics to melt in a reproducible manner suggests relatively straight-forward processes for joining and repair. Also the potential for recyclability of TPMC exists albeit as a chopped fiber, injection moldable grade material. The excellent damping characteristics of both TPMC and TSMC compared to all other structural materials suggest a real potential for reducing vibrations. The demonstrated use of polyphenylene sulfide (PPS) as a matrix for TPMC provides for a very low cost resin with a use temperature of approximately 100°C.

With respect to shortcomings the most frequently quoted problem is the poor compressive properties associated with TPMC. It has been argued that matrix modulus plays a dominant role in defining the compressive properties of composites. Since thermoplastics usually display modulus values 1/2 to 2/3 that of thermosets, it has been proposed that TPMC would display unacceptable compressive properties. However, in a recent paper by Budiansky and Fleck, they have indicated that fiber misalignment and matrix yield strength are far more important variables in controlling the compressive properties of polymer based composites. Hence, for the present one can greatly downsize the importance of the matrix modulus in limiting compressive properties.

A major corrosion problem associated with carbon fiber-epoxy matrix composites attached to aluminum has recently been identified. Presumably, the differences in EMF between aluminum and carbon promote rapid corrosion of the aluminum in the presence of moisture. Although not verified it would appear highly likely that use of TPMC would eliminate this problem, since many thermoplastics do not pick up moisture and in many cases also bond very strongly to the aluminum surface.

One area of need is to develop a TPMC which can be used for extended periods of time at 180°C (NASA's HSCT). Unfortunately, none of the resins which are available are able to meet this requirement. Even more serious, several companies currently engaged in design of high temperature matrices appear ready to pull out of this field. An important goal would be to design a resin which meets the needs for HSCT and costs under $10.00/lb (current cost of PEEK is approximately $145/lb).

Fiber Considerations

At present, carbon fibers (PAN based) represent the primary reinforcing agent currently in use in high performance composites. The likelihood that there will be a major change to a different fiber such as boron, BN or Al_2O_3 appears remote. On the other hand the cost of the carbon fibers at approximately $15/lb. will become more significant as the cost of manufacturing polymer matrix composites comes down. More important there are reports from Toray in Japan that indicate they are currently developing a $5/lb. carbon fiber. If this were to happen it would greatly accelerate transfer of this entire technology to Japan. There appears to be a need for tracking the work at Toray and for carrying out a cost analysis with respect to the manufacture of low cost carbon fibers.

Component Manufacturing

There was a unanimous view expressed by all of the participants in the workshop that the major area of need was the development of low cost/high reliability processes for fabricating TPMC's. It was also generally agreed that use of thermoplastics provides a potential for low cost manufacturing, design flexibility and decreased costs. However, there was limited experience concerning manufacturing/production, costs, and service.

On the positive side TPMC's can be processed without using costly autoclave and vacuum bag oven cures. TPMC's have been successfully fabricated into small parts using thermoforming, diaphragm forming and filament winding. Potential for cost effective fabrication of large structures appears possible for TPMC's but remains to be proven.

It is not surprising that progress on developing techniques for parts fabrication has been modest at best, since the Air Force program on component fabrication was initiated around 1987. The NASA program on the HSCT is still directed at developing a resin which will withstand 60,000/hrs at 170°C. Only recently have companies such as Quadrex or DuPont begun to develop a commercial business based on TPMC's. And this is being done at a time when the needs of DoD are being rapidly reduced.

There was at least one innovative development described by DuPont namely stretch forming using long discontinuous fibers (LDF); however such innovations represent the exception and not the rule.

Business Strategies

At present it is unclear which business strategy is uniquely qualified to insure survival in the highly competitive environment of the future. A company such as DuPont which has in the past been primarily a resin supplier is attempting to broaden its base of business by supplying composite parts. This approach insures participation in the higher value-added component parts business but brings the company into competition with its traditional customers. Dupont has also joined forces with Hercules and the University of Delaware in a broad program to evaluate composite fabrication using fiber placement. There are rumors that some of the traditional suppliers of thermoplastic matrices such as ICI and Amoco are planning to pull out of this business. Apparently Phillips has already sold its pre-pregging business on PPS to Quadrex. Several years ago Dow Chemical and Sikorsky established a joint business to develop advanced composites building on Dow's base in advanced resins and Sikorsky's skills in fabrication. This joint effort has barely been exercised in light of the recent downsizing of DoD needs.

Turning to the fiber manufacturers both BASF and Courtalds have ended their programs on commercialization of carbon fibers. Hercules, the leading manufacturer of carbon fibers in the USA is no longer profitable with the sharply reduced demand for carbon fibers. It is noteworthy that all of the carbon fiber that will be used on the Boeing 777 will be purchased from Toray. Perhaps one of the brightest lights on the horizon is the case of Quadrex which plans to sell several million dollars/yr of TPMC to Taiwan for use in the manufacture of tennis rackets.

Conclusions/Observations

1. Based on the talks presented at this workshop it appears clear that TPMC could provide improved performance characteristics over thermosetting matrices. Furthermore, they may be more compatible with future practices which will require recyclability and extended life usage. On the other hand the knowledge base for manufacture is limited to work carried out in the last five years. To maintain the necessary momentum to this field it would appear highly desirable to continue DoD programs aimed at component fabrication with the goal of retrofitting currently used component parts

which are especially liable to damage or corrosion.

2. ARPA should take the lead with respect to other government agencies such as NIST, NASA, DOE and the respective DoD agencies to establish a set of goals which address both DoD and commercial needs for all polymer matrix composites. Specific directions might include:

   - Automating component parts fabrication based on existing processes.
   - Developing a data base on performance which permits a predictive capability in design of component parts.
   - Exploring new concepts for rapid, low cost fabrication of TPMC and TSMC.
   - Pursuing development of semicrystalline thermoplastics which have the potential for 1) a general purpose, low cost resin matrix and 2) display excellent high temperature properties for use in DoD applications and for the HSCT.
   - Establishing feasibility to manufacture much lower cost carbon fibers e.g. $5/lb.

3. To sustain development of both TPMC and TSMC through a period of major downsizing by both DoD and industry some thoughts should be given to establishing a major center which would have as its primary goals the issues of manufacturability and affordability. Such a center would also support establishment of a data base on performance characteristics of TPMC and TSMC. Other activities that might be considered would involve small exploratory studies on advanced matrices and fibers.

4. To enhance the commercial development of polymeric composites government agencies should encourage the formation of new businesses via SBIR, precompetitive consortia....

* *The participants in this workshop were drawn primarily from groups who have been strong advocates of TPMC versus TSMC. Hence, there may have been a bias in the presentations that was slanted toward TPMC. In the section on Conclusions/Observations an attempt is made to treat these respective areas as one common theme namely polymer matrix composites.*

THERMOPLASTIC MATRIX COMPOSITES (TPMC)

James Economy

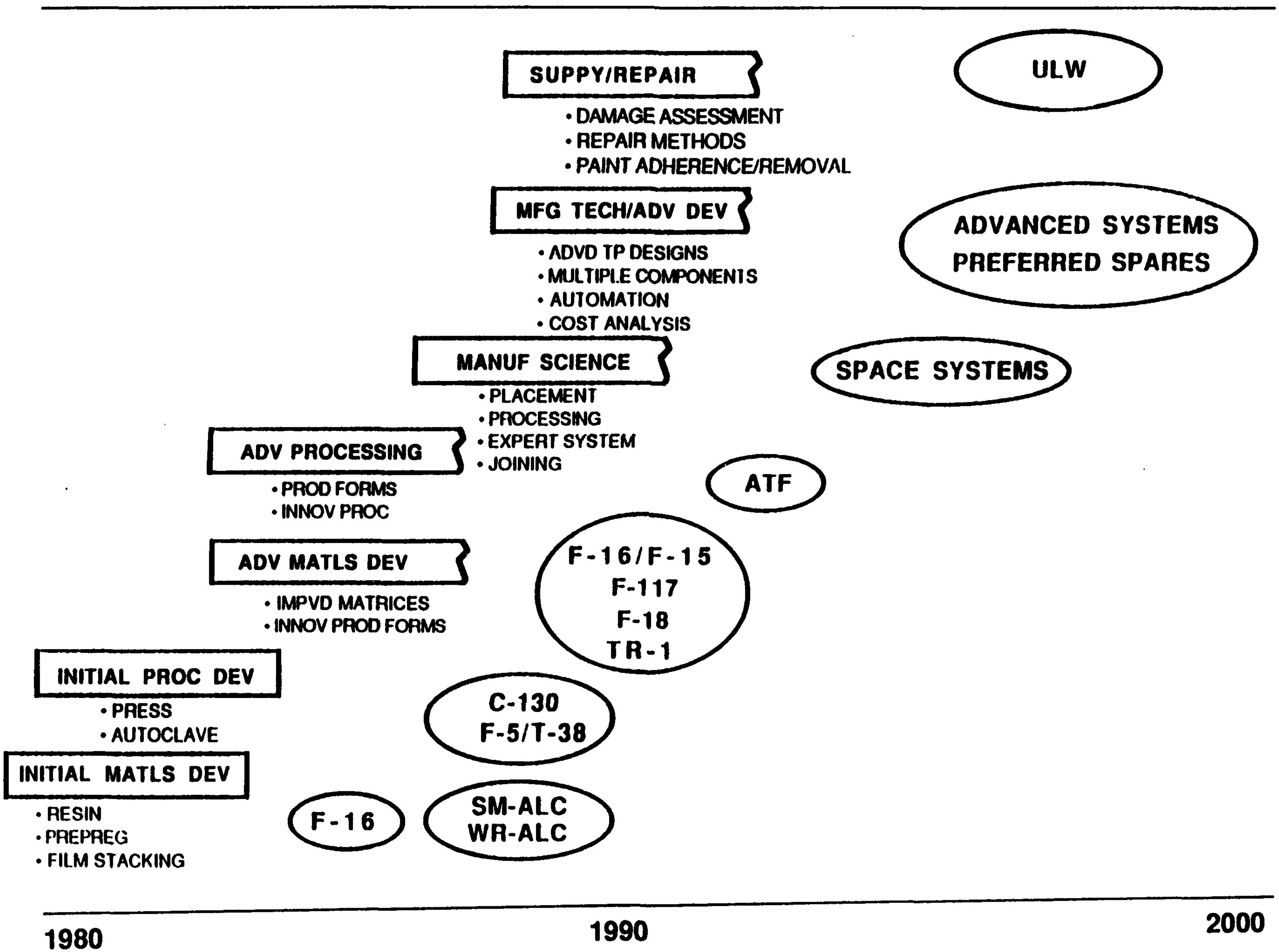
Objective

- Assess current status of TPMC
- Examine future R&D needs
- Explore strategies for sustaining commercial development

DoD Relevance

- Polymer matrix composites already fulfill a number of critical needs for DoD
- TPMC may offer advantages for future prototype development programs as well as for insertion in existing uses
- Increasing emphasis by DoD on recyclability and life extension of military hardware may argue for accelerated development of TPMC

TP COMPOSITE EVOLUTION



Scientific and Technological Issues

Current Status of TPMC

- Good translation of mechanical properties
- Composites display excellent damage resistance
- Simplified joining and repair demonstrated
- Poor compressives may not be a problem
- Some TPMCs display superior thermooxidation resistance
- Low moisture pick-up

Potential to Design TPMC for:

- Recyclability
- Creep resistance at 180°C
- Low cost manufacture
- Resistance to stress corrosion
- Compatibility with metal attachments

Scientific and Technological Issues (contd.)

Manufacturing/Affordability of TPMC

- Very limited history — ~5–6 years
- Parts demonstrations by Air Force on eight aircraft
  - — Technology base established
  - — Secondary structures/repairs - demonstrated
  - — Limited manufacturing experience/cost data

Business Strategies

- Resin developers
- Fiber manufacturers
- Forward integration into parts business
- Pre-preggers
- Consortia: Dow/Sikorsky
  DuPont/Hercules/U of Delaware

Conclusions and Observations

- Ecumenical approach to polymer matrix composites
- Coordinated program defined by government/industry to address both DoD/commercial opportunities
- Primary emphasis on manufacturing
- Need for a major center on polymer matrix composites
- Facilitating a proliferation of small business thrusts

THERMOPLASTIC MATRIX COMPOSITE

Workshop Coordinator: James Economy

July 22, 1993

8:00 am	Opening Comments, J. Economy (DSRC/University of Illinois)
8:10 am	Introduction, J. DeVault (ARPA)
8:30 am	"Background & Overview of Thermoplastic Composites," T. Benson-Tolle (Wright-Patterson)
9:20 am	"High Performance Thermoplastic Composite Materials & Applications," J. Ogonowski (McDonnell Douglas)
10:00 am	Break
10:20 am	"Cost Effective Thermoplastic Applications," R. Ramkummar (Northrop)
11:00 am	"Aerospace Thermoplastics/Future Needs," G. Wood (Oak Ridge)
11:40 am	"Future Directions in Thermoplastic Composites," N. Johnston (NASA Langley)
12:20	Lunch
1:20 pm	"Initiative in Cost Effective Fabrication Technology for Thermoplastic Composites," M. Lamontia (DuPont)
2:00	Five short presentations: C. Crowe (Amoco), J. Mondo (Quadrex), J. Economy (U. of Il.), R. McCullough (U of DE), Alan Miller (Lockheed)
2:50 pm	Break
3:05 pm	Discussion

THERMOPLASTIC MATRIX COMPOSITES

July 22, 1993

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CROWE, Christie	Amoco Perf. Prod.	404-772-8372
DE VAULT, Jon	ARPA	703-696-2296
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FREUND, Ben	DSRC/Brown	401-863-1476
HEUER, Arthur	DSRC/CWRU	216-368-3868
HIRTH, JOHN	DSRC/Wash. State Univ.	509-335-8654
HOPPS, John	NSF/DMR	202-357-9794
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JOHNSTON, Norman J.	NASA Langley Res. Ctr.	804-864-4260
LAMONTIA, Mark A.	DuPont Adv. Matl. Systems	302-733-8821(8854F)
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LYTIKAINEN, Bob	ARPA	703-696-2242
McCULLOUGH, R.	Univ. of Delaware/CCM	302-831-2310
MILLER, Alan K.	Lockheed R&DD	415-424-2583
MONDO, Jim	Quadrax	401-683-6600
OGONOWSKI, Jim	McDonnell Douglas	314-234-3458
POESCH, Jon G.	Hercules, Inc.	801-251-3105
RAMKUMAR, Ram	Northrop Aircraft Division	310-331-7102
RAPP, Robert	DSRC/Ohio State Univ.	614-292-6178
SATER, Janet M.	IDA	703-578-2978
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FUNCTIONAL ORGANIC AND ORGANOMETALLIC MATERIALS

Frank DiSalvo and George M. Whitesides

EXECUTIVE SUMMARY

Workshop Objective

The objective of this workshop was to survey organic and organometallic materials for new properties, and to identify concepts in molecular or electronic structure leading to materials with unique properties.

Relevance to DoD

Defense systems of all types are dependent on the properties of the materials from which they are made. Historically, the DoD has been the most important sponsor of research leading to the development of advanced materials in the U.S. With the end of the cold war, the need for the development of higher-performance generations of traditional military systems—attack aircraft, tanks, ships—is less urgent than it was in the 1970s and 1980s. A new series of requirements focused on collection and manipulation of information, on rapid and flexible response, on supporting small units and individual soldiers, and on cost containment, has emerged as important. These new requirements will require new materials. In addition, the concept of "national security" now sees military capability and civilian economic capability as being inextricably connected. Practical constraints — cost, environmental compatibility, potential for generating jobs, opportunity for commercial spin-off — are increasingly important in military systems.

There is a heavy emphasis in planning the DoD research investment to focus on technology that can be commercialized in the relatively short term, and preferably on technology that can benefit from interaction with the commercial sector (either by adopting commercial components and systems, or by spinning off technology into the commercial sector). A strength of the U.S. system has, however, always been its prolific creativity. Although the shift in emphasis from discovery to development in the U.S. RD&E activities is un-

doubtedly healthy for the country, it should not proceed to the point where discovery is forgotten. The discovery of new materials—that is, materials with genuinely unique properties—would still be of great advantage, both militarily and commercially, provided that these materials fell in categories whose properties could be used. The objective of this workshop was to survey a rapidly developing area of materials science—organic and organometallic functional materials—to determine what areas are most promising for current commercial development, and what areas offer substantial promise of delivering useful new materials in an exploratory research program.

Scientific & Technical Summary

Geoff Ozin (University of Toronto) An important subject at the border between chemistry and physics is the properties of meso-scale (1 to 100 nm) objects. Manufacturing at the lower end of this range of sizes is difficult, and new methods are needed if nano-structured materials are to become practically important. Ozin described two new methods of synthesis for meso-scale systems. The first was a series of procedures for making structurally well-defined clusters (especially of semiconductor materials) in the pores of molecular sieves. The second was extensions of methods of making sieves (typically aluminosilicates or phosphates) to sieve-like structures of electronically functional materials. These projects (carried out in collaboration with Union Carbide Corporation) offer attractive routes to materials that consists of well-defined void channels and cavities, either containing electronically functional materials, or composed of electronically functional materials. Related work is going on in other laboratories in the U.S., and the field of zeolite-enclosed and zeolitic semiconductor systems is one with real promise to make new materials.

Among the interesting applications of these methods was the synthesis of zeolites containing Si_8 clusters (which apparently photoluminesce), and of Sn/S/Se-based porous materials whose electronic properties changed with the character of the molecules included in their pores.

The synthetic techniques outlined by Ozin offer a important new route to nano-materials, with advantages and disadvantages. The advantages are that these processes are scalable to substantial quantities, and that they produce new materials with potential applications as light emitters and sensors. The disadvantage is that there is no obvious strategy at the instant to address individual nanoparticles, and that they are produced only in regular arrays; they do not,

therefore, seem to be immediate candidates for small-scale electronic devices.

Among the interest features of these systems is the fact that the particles included in the cavities are often somewhat smaller than the cavities, and thus able to "rattle" inside the cavity. The frequency and effect of this rattling has not been explored, but it is a new type of dynamic behavior in materials, and may provide the basis for new properties.

Art Epstein (Ohio State University) reviewed the field of molecular magnets: that is, of molecular materials showing ferro- or ferrimagnetic properties. This is a field in which there has been explosive advance in the last years: Curie temperatures have increased from a few Kelvin to a value for one compound — $V(TCNE)_x(CH_2Cl_2)_y$ — well above room temperature. Most other compounds in this class still have a $T_C < 200°K$, and more research is required to understand the relation between structure (especially 3D structure) and properties in order to make additional members of the high T_C class. Unfortunately, the competition for these new ferromagnetic organic materials comes from older materials such as magnetite and iron, and it seems unlikely that the organometallic magnets—usually pyrophoric charge transfer salts of metals or metallocenes and acceptors such as tetracyanoethylene — will compete on either cost or ease of manufacturing. These materials are a fundamentally new class, but there are no clear technological targets for them yet.

Epstein appropriately pointed out the analogy between organic ferrimagnets and organic conductors. It required a number of years of research to find the proper niche for the latter (in light-weight, flexible batteries); a similar effort will be required for the organometallic magnets, for which applications are not immediately obvious.

Frank DiSalvo (Cornell) emphasized the structural difference between solid-state organic chemistry and inorganic chemistry. Organic materials have electronic structures that are relatively predictable, and in which the weak interactions between molecules make substitution and modification relatively simple. It is, at present, much more very difficult to predict the properties of inorganic materials. Interactions between atoms can be very large, and the range of accessible structures is also large. Although most electromagnetically functional materials are now inorganics (metals, semiconductors, metal oxides and sulfides), predicting new materials with new properties is essentially impossible. Research must therefore proceed with a strong element of empiricism and discovery. A useful predictive structure for solid-state inorganic chemistry

would be enormously useful. It would also be very useful to build a base for predicting and controlling structure and properties of organic materials, especially in three dimensions. A key to solid-state chemistry and in connecting it to materials is three-dimensional structure and properties.

Tobin Marks (Northwestern) discussed the application of self-assembled multilayer films (especially those covalently cross linked through siloxane groups) in the fabrication of optically functional materials. It is clear that the cross linked, self-assembled system have much greater stability than most polymer systems, and that they may, in fact, be legitimate candidates for use in optical systems. Good targets suggested were solid state light emitters in the blue consisting of a semiconductor diode laser coupled to an organic thin-film frequency doubler, and photorefractive systems with thickness of ca. 100 µm built up from multiple oriented monolayers.

Tom Mallouk (University of Texas) described a number of methods for making multilayer materials systems, and applications for these systems. Zirconium alkanephosphonates offered routes to controlled-pore layered solids, and thus to molecule-specific sensors. Electrochemistry offered the opportunity to electrodeposit controlled thin films of metals and metal oxides. A large number of clay materials can be obtained in layered form: these can, in principle, be exfoliated and reconstituted to form new materials classes.

Edel Wasserman (DuPont) described studies with C_{60} and related materials. The particular type of chemistry exploited in these studies was the characteristic reactivity of these materials toward organic free radicals. It is possible to add up to eight CF_3 groups to C_{60}, for example. These derivatives of C_{60} apparently are being considered for commercial applications within DuPont. One application might be as a cross-linking agent for polymers prepared by free-radical polymerization.

Conclusions and Observations

Issues in the Development of New Materials

The commercialization of new materials has always been a difficult task: they typically constitute only a small part of the final, assembled system, and the process of justifying the value they add to a complex system is not well worked out. New materials for structural applications also have the disadvantage that they must compete on the basis of price with existing materials, and that reducing the price of a structural material requires justifying very large

scales of production (in order to achieve the economies of scale). Materials to be used in electronic applications have a difficult time, but the requirements in cost per pound are less stringent.

One instance in which it is relatively straightforward to introduce a new material is when that material brings unique characteristics and properties. In this circumstance, justifying a high initial price may be simpler for a user (since it may lead to a new class of materials) than it would be if the materials were being considered as a substitute for an existing commodity material. A focus on new materials with unique properties applicable to electronics, optics or related areas thus seems practical and justifiable. (New materials for applications in biology and medicine is another attractive area in which to try to discover new materials; this area falls outside of most of the interests of ARPA).

Nanostructures and Quantum Dots

One class of plausible applications is in the synthesis of semiconductor nanostructures with better structural definition and greater stability than those provided by colloids and other non-enclosed systems. These types of systems are of great interest for their potential in band-gap engineering, and they may be useful as light emitters. For zeolitic structures that are themselves semiconducting, there is a potential for the development of systems whose electronic response is modified by the reversible inclusion of adsorbates; such systems might be useful as sensors.

Molecular Magnets

The most important issue with molecular magnets is to begin to consider their properties in the light of possible applications. Existing systems have no immediate applications, but the development of the field has been so rapid, and the potential for tailoring the properties of these materials through synthesis is so large that intuition indicates that there must be applications. The highest Curie temperature — >300°K — is so far an isolated compound, and better understanding of its properties may help predict new materials with high values of T_C. If these organic/organometallic magnets will always require encapsulation to protect them from oxidative destruction, all applications will obviously have to be compatible with that limitation.

Optical Systems

Several of the speakers emphasized the flexibility with which organic structures can be modified to tailor their optical properties, and the useful

measure of predictive capability provided by current theory. The optical properties of organics and organometallics are clearly complementary to those of semiconductors: for example, it is very difficult to get efficient production of blue light from semiconductors, but relatively straightforward for organics. Organics generate red light with difficulty; for semiconductors, emission in the red is common. Both Ozin and Marks made strong cases for a program in using organometallics to make optically functional materials—zeolite-enclosed semiconductors fabricated starting with organometallic precursors, and multilayer self-assembling systems for non-linear optics and for photorefractives. The key unanswered question about organic materials in this context is their stabilities over long periods. Liquid crystal displays to, however, provide a successful application of organic materials in an electro-optical systems with high requirements for operating lifetimes.

Carbon: C_{60} and Buckytubes

The importance of these new forms of carbon remains to be established. One important issue is cost: even in significant volume, their cost will probably be $1,000–$10,000 per pound (by contrast, Buckytubes — long, small graphitic tubes — can probably be produced for <$5 per pound). It is clear that C_{60} has reactivities characteristic of a highly reactive polyolefin, and its tendency for cooperativity in reaction may be interesting. It is not clear that it can be produced inexpensively enough to be used in larger volume applications. Even if it does become a valuable new chemical entity, there is, so far, no clear hint that it will have revolutionary impact on materials science. The new forms of carbon are, however, still sufficiently early in their development that there could be important surprises waiting to be made, both in synthesis and in reactivity and properties.

Discovery of New Materials

The pace of discovery in the area of functional organic and organometallic materials is now very rapid: the solid state and "chemistry of/for materials" is a fashionable and productive area which has attracted substantial talent. Several types of capability would improve the efficiency of the field. First, and most important, is better coupling of synthesis (usually done by chemists) to measurement and applications (usually carried out by physicists, materials scientists, and engineers). The second is improved capability to model three-

dimensional structure and properties; this capability is not yet available, but the current of computation offered by massively parallel and RISC machines may be sufficient to move the field to a predictive plateau. Third, clear definition of areas in which new materials would be accepted (that is, in which it seems genuinely implausible that existing materials can solve the problem) would help to focus research. Finally, continuing financial support that at least tolerates exploratory work in synthesis and properties of materials is essential. Much of this work is being cut back in the present focus on relevance.

Applications

Within the context of ARPA programs, there are several opportunities for applications of the types of materials discussed in this Workshop.

Sensors

Both the zeolitic materials of Ozin and the layered materials of Mallouk may form the basis for molecule-specific gas sensors. These could be used in the developing systems for military medicine as non-invasive breath analyzers, and also may be applicable to problems in CBW and, perhaps, in explosives monitoring in counter terrorist technology.

Electronics

If it were possible to grow zeolitic structures as two-dimensional crystals, and to then grow the encapsulated semiconductors inside them, they might be applicable in some of the advanced concepts being discussed in the Ultra program.

Manufacturing

Self-assembly is a strategy that may be useful in providing surface coatings—for passivation of electronic materials during processing, and perhaps for corrosion protection. These types of applications should be considered in the context of lifetime extension programs for aging platforms and systems.

Structural Materials

Wasserman made the point that the most facile introduction of new materials into structural systems comes as modifications of existing systems. The application of C_{60} in modifying the properties of polymers is one example. Layered clays and buckytubes as components of microcomposites is another.

FUNCTIONAL ORGANIC AND ORGANOMETALLIC MATERIALS

G. Whitesides and F. DiSalvo

Objective of the Workshop:

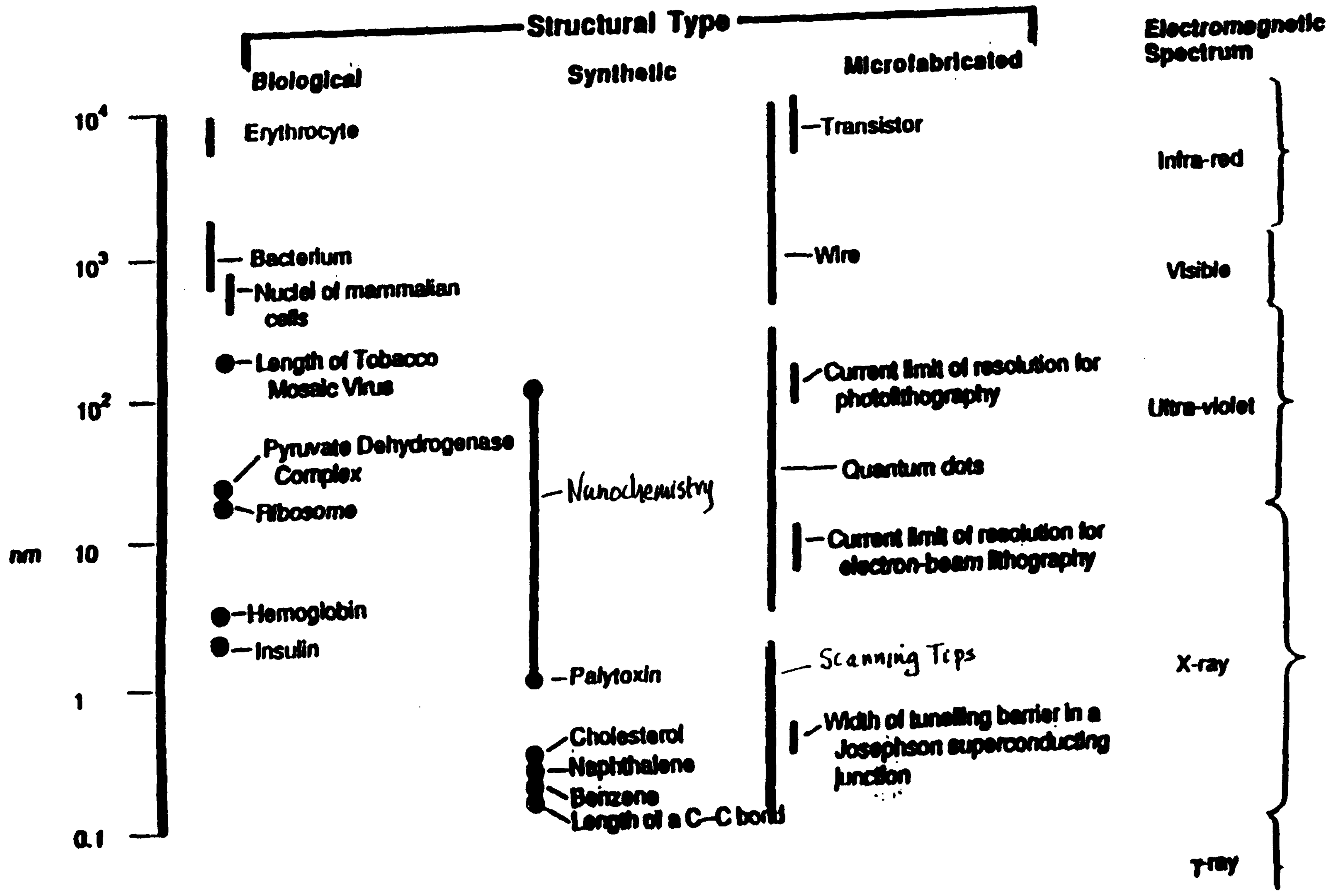
- To survey organic and organometallic materials for *new* properties.

$$\text{Value} = \frac{\text{Benefit}}{\text{Cost}}$$

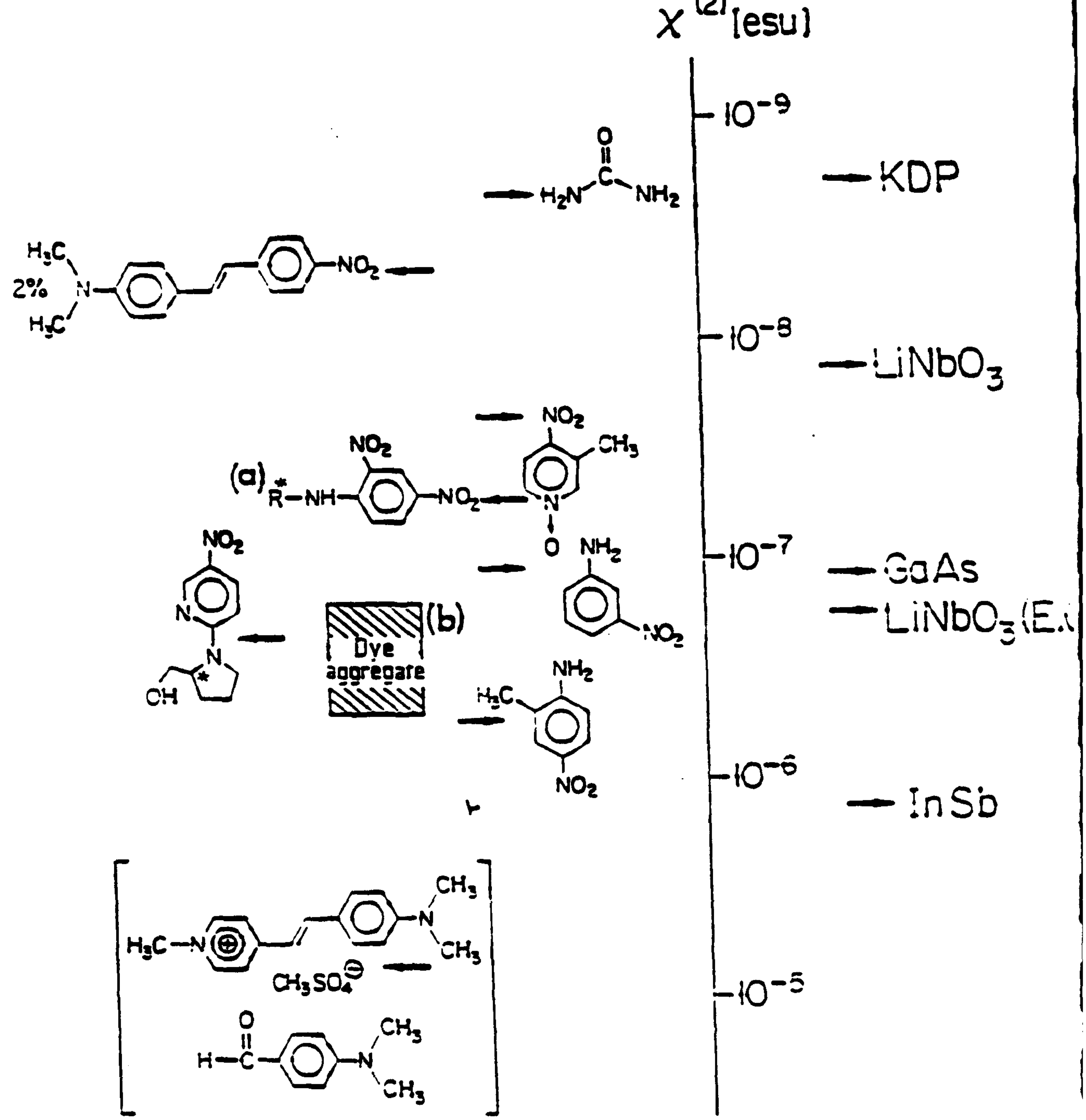
DoD Relevance:

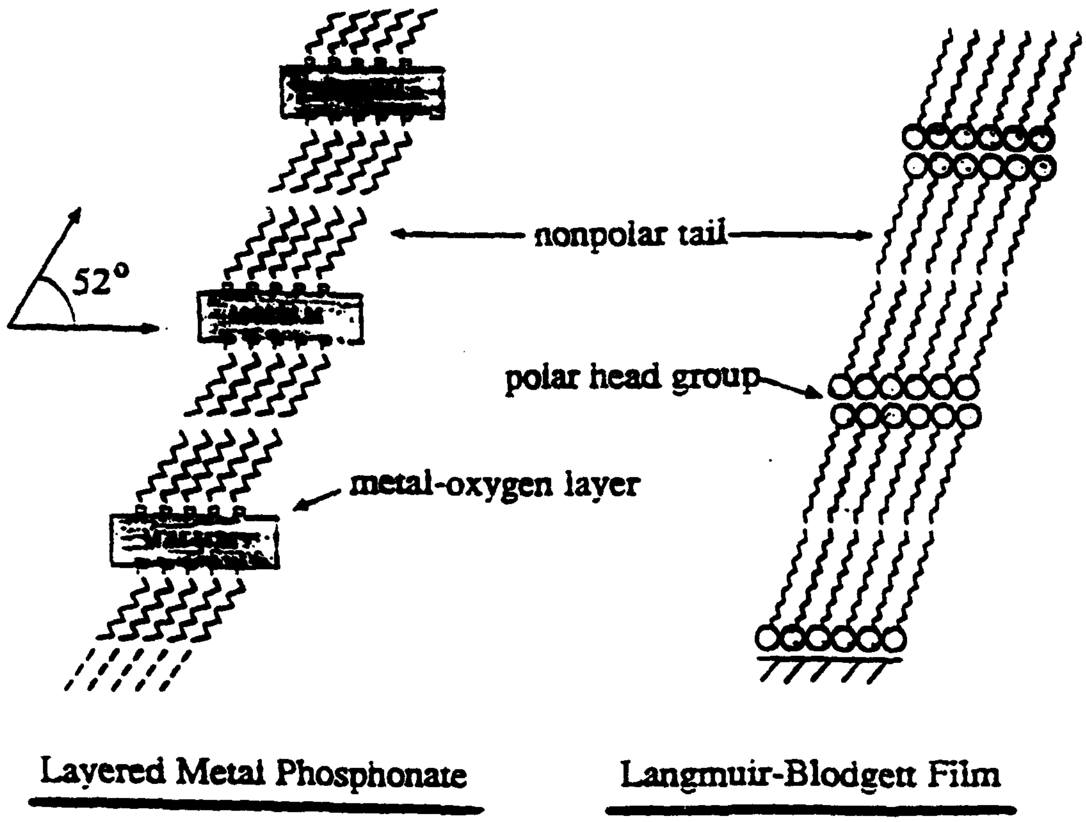
- Unique properties offer unique capabilities
- Organic materials are easily manufactured, light-weight, non-metallic. (Examples: organic polymer conductors, liquid crystal displays, high-strength polymers, ferrofluids).
- Relevant to specific ARPA problems:
  - Blue light emitters
  - Molecule-specific sensors for military medicine
  - Photorefractives for optical memories
  - Surface passivating layers: manufacturing,corrosion, lubrication
- Manufacturable semiconductor nanostructures

A Comparison of the Relative Sizes of Structures Generated in Biology, Synthetic Chemistry and Nanofabrication

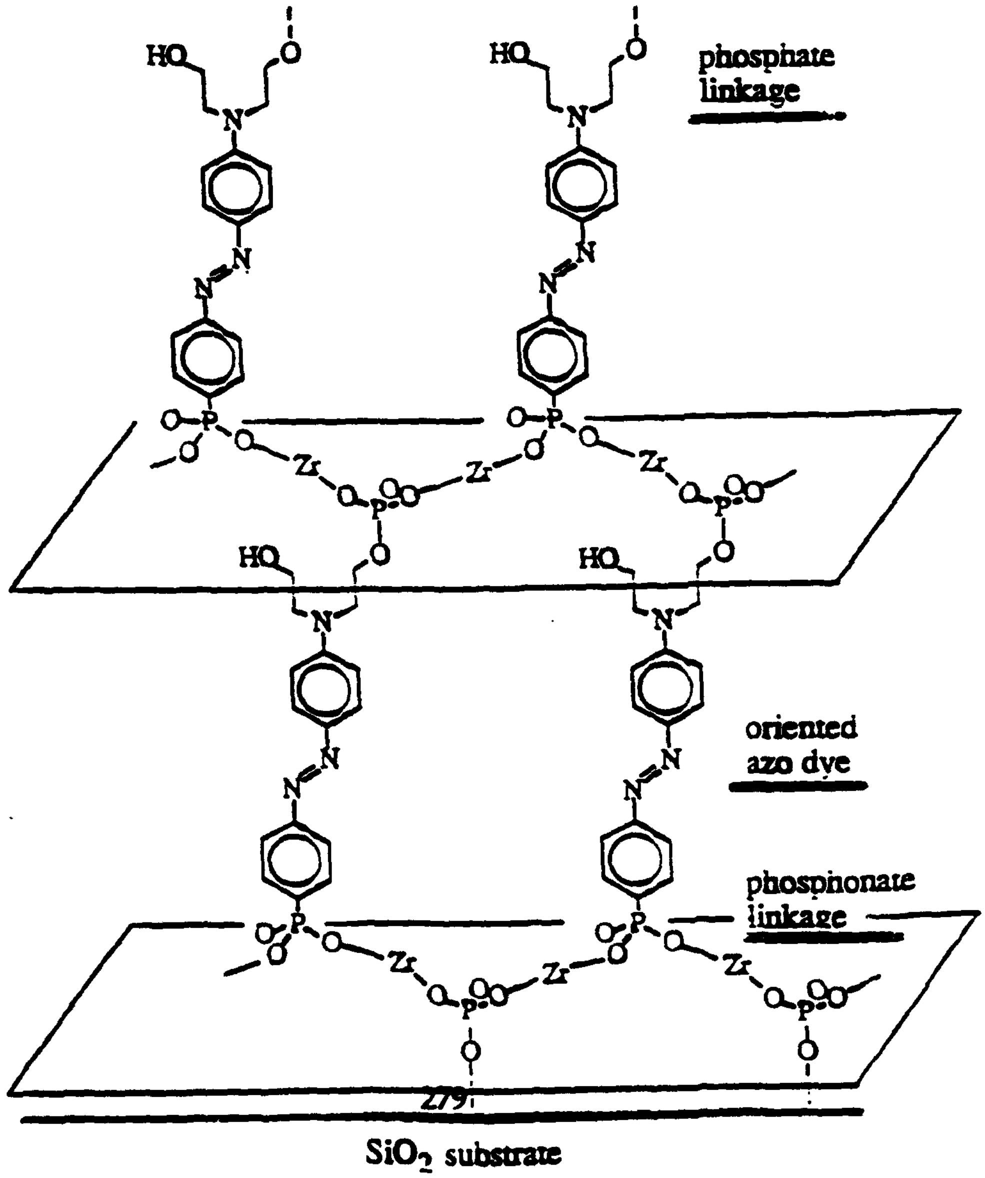


COMPARISON OF MOLECULAR AND CONVENTIONAL INORGANIC MATERIALS

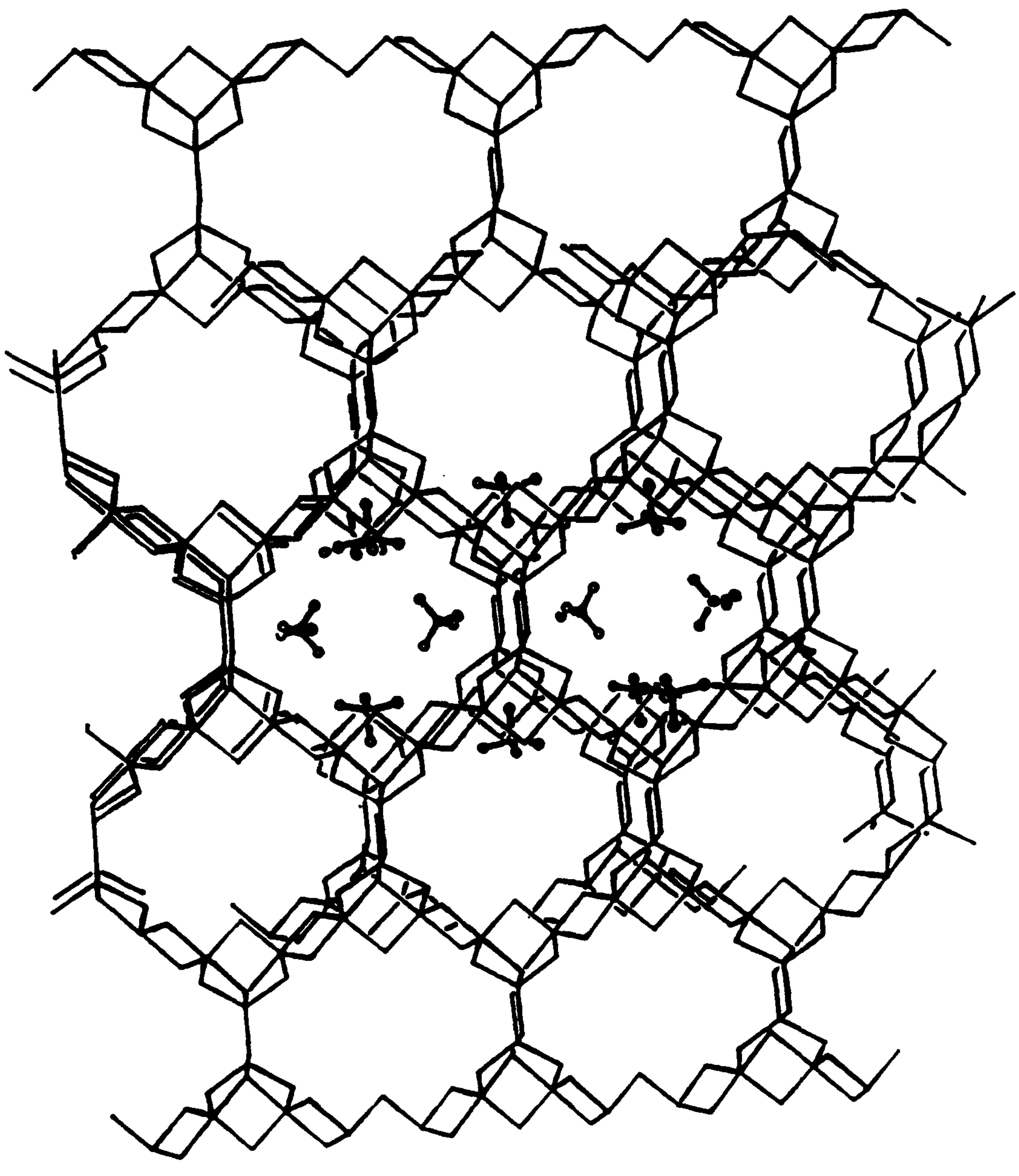


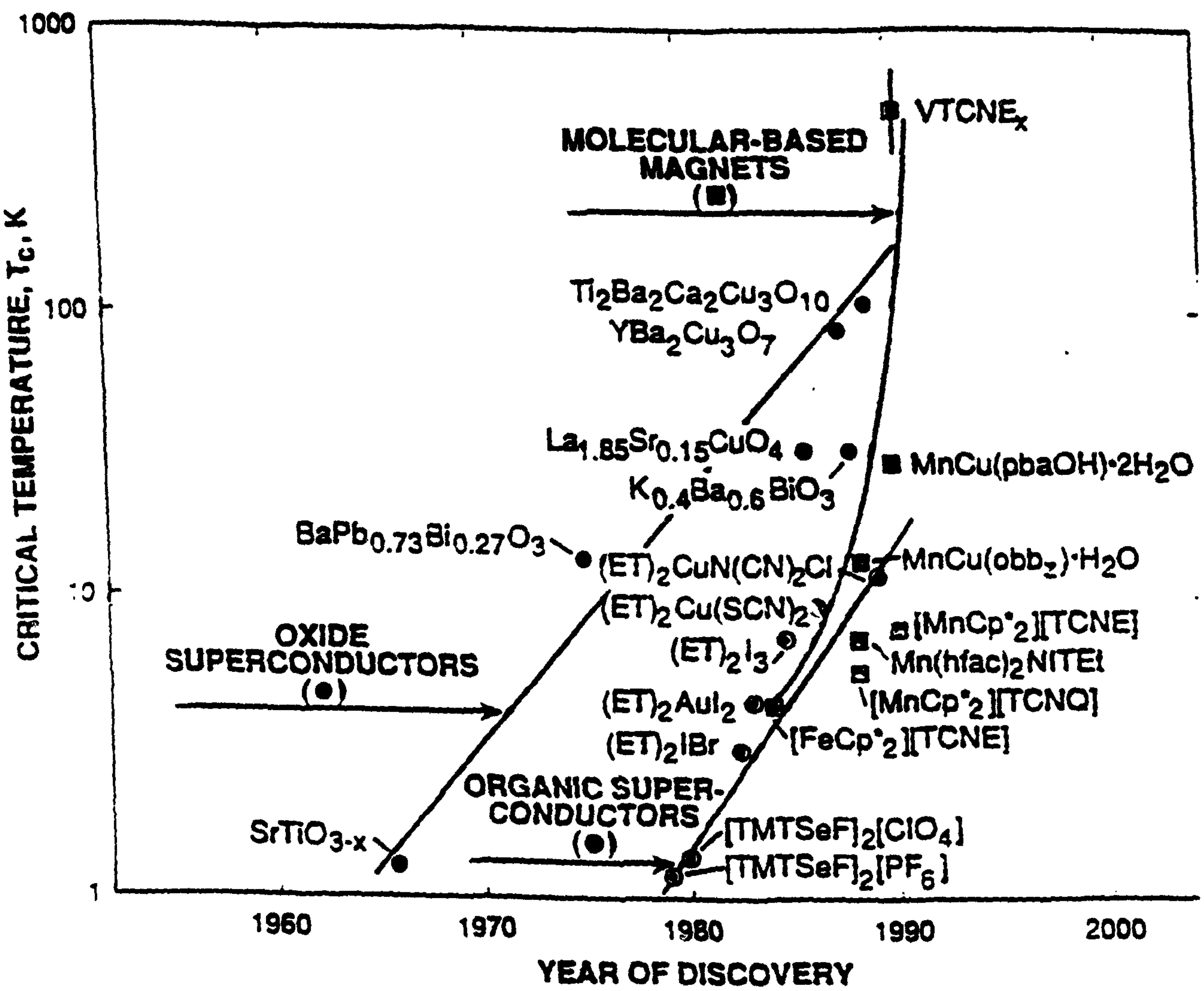


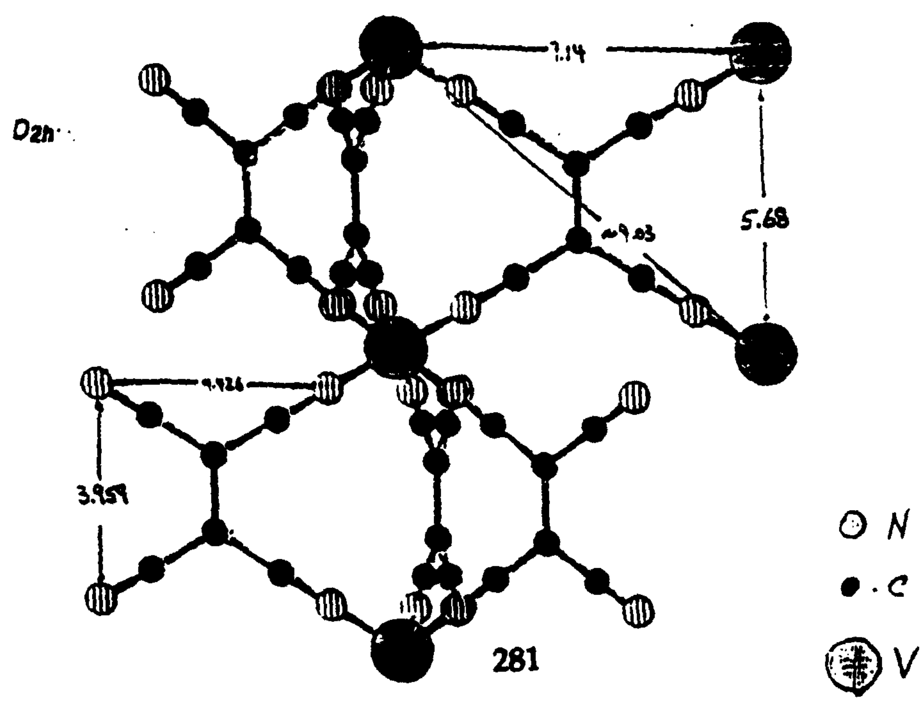
nonpolar tail
52°
polar head group
metal-oxygen layer
Layered Metal Phosphonate
Langmuir-Blodgett Film



HO
O
N
P
Zr
phosphate linkage
oriented azo dye
phosphonate linkage
SiO2 substrate




CRITICAL TEMPERATURE, Tc, K
YEAR OF DISCOVERY
1000
100
10
1
1960
1970
1980
1990
2000
MOLECULAR-BASED MAGNETS (■)
OXIDE SUPERCONDUCTORS (●)
ORGANIC SUPER-CONDUCTORS (●)
VTCNEx
Tl2Ba2Ca2Cu3O10
YBa2Cu3O7
La1.85Sr0.15CuO4
K0.4Ba0.6BiO3
MnCu(pbaOH)·2H2O
BaPb0.73Bi0.27O3
(ET)2CuN(CN)2Cl
MnCu(obbz)·H2O
(ET)2Cu(SCN)2
[MnCp*2][TCNE]
(ET)2I3
Mn(hfac)2NITEt
[MnCp*2][TCNQ]
(ET)2AuI2
[FeCp*2][TCNE]
(ET)2IBr
SrTiO3-x
[TMTSeF]2[ClO4]
[TMTSeF]2[PF6]


D2h
7.14
5.68
9.03
9.926
3.959
N
C
V

FUNCTIONAL ORGANIC MATERIALS

Workshop Coordinator: George M. Whitesides

July 23, 1993

8:00 am	Introduction to the Workshop, George Whitesides (DSRC/Harvard University), Frank DiSalvo (DSRC/Cornell University), Bob Crowe (ARPA)
8:15 am	"New Materials", Geoff Ozin (University of Toronto)
9:30 am	Break
9:45 am	"Organic and Organometallic Ferromagnets", Art Epstein (Ohio State University)
10:30 am	"Solids with Novel Properties and Structures", Frank DiSalvo (DSRC/Cornell University)
11:15 am	"Design of Molecule-based Electrooptical Materials", Tobin Marks (Northwestern University)
12:00 Noon	Lunch
1:00 pm	"Solid-State Chemistry", Tom Mallouk (University of Texas)
1:45 pm	"Carbon-Based Systems", Edel Wasserman (E. I. duPont de Nemours & Co.)
2:30 pm	Summary and Discussion
3:30 pm	Adjourn

FUNCTIONAL ORGANIC AND ORGANOMETALLIC MATERIALS

July 23, 1993

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EPSTEIN, Arthur J.	Ohio State Univ.	614-292-1133
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ARPA/DSRC WARGAMING

R.C. Lytikainen

EXECUTIVE SUMMARY

In the second year of our "wargaming" project, Advanced Research Projects Agency (ARPA) program managers and Defense Sciences Research Council (DSRC) scientists are deriving considerable benefit from participation in and observation of military wargames, exercises and site visits. Even as major powers are downsizing and attempting to convert defense spending into commercial investment, the Cold War is being replaced by regional, geopolitical, religious and ethnic conflict. Via our wargaming visits, we have a birds eye view of contemporary, evolving military thinking and are gaining insight into better military application of new technology.

There is no substitute for first hand appreciation of new concepts of warfare (e.g. the Navy's "From the Sea" and the Air Force's "Global Reach"), for understanding of rapid deployment/employment force operations (e.g. Maritime Preposition Force/MPF, hi-speed Landing Craft, Air-Cushioned/LCAC, Carrier Battle Group, etc.), nor for knowledge of the challenges of littoral warfare (amphibious and mine warfare) and regional peacefare (e.g. Lebanon, Cambodia, Bosnia and Somalia).

We are building linkages with the military and are working closely with the Navy's "Naval Science Assistance Program (NSAP)", the "Scientist-to-Sea" and the Air Force's "Blue Two" programs, visitation projects which expose our materials, and electronics scientists and engineers to real military application and environmental problems that need near/mid term solutions. We are also learning that in an era characterized by the prospect of virtually no additional bucks for new systems, we still need to have the bang. Much of this bang will apparently have to come from life extension of aging systems, from more focused R&D, from early concept demonstration and rapid prototyping, and from better simulation, modeling and wargaming.

ACTIVITIES

21 DSRC scientists and 22 ARPA program managers participated in a wide variety of military wargames, exercises and other military installation visits since the 1992 DSRC Summer Conference (a total of 57 and 58 trips, respectively). In addition, three Office of Naval Research program managers joined us for four different events, for a total of 25 wargame, 41 exercise and 84 installation person-visits, summarized below (details on following pages):

Wargames

- Naval War College, Newport, RI	"Global War Game-92"
- Air Force War College, Mongomery, AL	"Global Reach-92"
- Naval War College, Newport, RI	"SEACON92"
- Naval Strike Warfare Center, Fallon, NV	"Carrier Air Wing 2-93"
- Naval Amphibious Center, Coronado, CA	"Sri Lanka NEO-93"

Exercises

- Marine Corps, Camp Pendleton, CA	"Tandem Thrust"
- Marine Corps, 29 Palms, CA	"Combined Arms Ex"
- Army Training Center, Ft. Erwin, CA	"OPFOR"
- Coalition/Joint/Marine Corps, Kuwait	"Native Fury-93"

Military Installations/Activities

-Tinker Air Force Base, Oklahoma City, OK	Aircraft Maint/Rework
- Marine Corps Air Station, Cherry Point, NC	Aircraft Maint/Rework
- NAS/NADEP/AIMD, Norfolk, VA	Aircraft Maint/Rework
- NORAD, SPACECOM, Colorado Springs	CINCSPACE, AFSCN
- Naval Air Station, Whidby Island, WA	EW/EA6B, Attack/A6
- Aircraft Carriers in-port, North Island, CA	USS Ranger, Kitty Hawk
- Nuc Attack Subs in-port, Point Loma, CA	USS Chicago, Topeka
- Deep Submergence Unit, North Island, CA	DSRV/DSV/UMV
- NADEP, North Island	Aircraft Maint/Rework

Specific actions have been undertaken by ARPA/DSRC members as a result of our getting closer to the military customer. Some of these include:

• Several Defense Sciences Office (DSO) and Electronic Systems Technology Office (ESTO) R&D programs have a Marine Corps customer (Commanding General, 1st Marine Force/CGIMEF) ready and willing to work

with ARPA program managers to do concept demonstrations in a desert environment at 29 Palms, CA. Technologies we are maturing and looking to test over the next year or two include; portable/mobile photovoltaics, battlefield management and display, low-power communications/positioning devices, superconductivity technology, fuel cell and battery technology, and head-mounted displays.

• A "Life Extension of Aging Structural System" workshop (reported on elsewhere in this report) at this year's Summer Conference, was a direct result of meetings held with the Navy on "H46 Helicopter Rotor" problems during last year's conference, as well as discussion with military service air rework people during the year.

• An initiative has begun with the Commander, Naval Air Pacific (COMNAVAIRPAC) in the hazardous material (HAZMAT) disposal and control area as a result of our visit to the USS Kitty Hawk (CV-63) this summer. The Navy has a significant HAZMAT problem during their several month at-sea deployment cycle (with all their ships), which we think ARPA/DSRC might be able to help them with.

• The first successful Grunion Hunt in 26 years of DSRC summer meetings, was concluded in the early morning hours of 22 July 1993 (0030 PDT) at San Diego's Ocean Beach, with the capture of an 8" live specimen of ***Leuresthes Tenuis*** (also known as "silversides").

CONCLUSIONS AND OBSERVATIONS

The ARPA/DSRC wargaming project continues to be highly successful in "building an intuition" in our scientists and program managers. A quote from one of our ARPA program managers seems to best sum-up it's success:

"(We) now have a new set of priorities. Before,...talked about architecture, bits, multichip modules, throughput, etc. Now...are talking about ruggedness, reliability, repairability, friendly interfaces, and a variety of operational uses. It would be difficult to overstate how important these little visits are to us and in the longer term - to the Marines."

–Dick Urban/ESTO, May 1993

WAR GAMES

R. Lytikainen

30 July 1993

WARGAMING

(Expose ARPA/DSRC to Military Operations & Decision Making Process)

- **CHANGING WORLD**
- **GAIN INSIGHT-MILITARY APPLICATION OF TECHNOLOGY**
- **BETTER BANG FOR THE BUCK**
- **LINKAGES/BUILDING AN INTUITION**

30 July 1993

LESSONS LEARNING

- WORLD STILL CHANGING

- GAINING INSIGHT
  - New Concepts of Warfare ("From the Sea", "Global Reach")
  - Rapid Deployment/Employment (MPF, LCAC)
  - Littoral Warfare (amphib., mine warfare)
  - Littoral Peacefare

- BANG FOR LITTLE OR NO ADDITIONAL BUCKS
  - Life Extension vs New Systems

- LINKAGES BEING BUILT
  - NSAP (ARPA-VLAP)
  - "Scientist to Sea"
  - Blue Two

- INTUITION BEING BUILT
  - Talk to the people, experience the environment & look at the stuff they use

- NEED MORE/BETTER SIMULATION, MODELING, GAMING, CONCEPT DEMONSTRATING, RAPID PROTOTYPING

30 July 1993

MARINE CORPS CAX/ARPA CONCEPT DEMONSTRATION
(Sep 93-Aug 94)

• Battlefield Management/Display Technology (in Humvee/LAV)	Urban
• Photovoltaics Applications (mobile)	Barker
• Head-mounted Displays ("Navigator") (low-level helicopter ops to maintainence mechanics)	Gabriel
• Low-power Comm/Positioning Devices (recon troops) ("Pathfinders")	Urban
• Fuel Cell/Battery Technology	Loda

30 July 1993

OBSERVATIONS/REMARKS

- "Remarkable training, motivation, knowledge and focus of young officer and enlisted personnel"
- "High level military decision makers are positive about our interaction with them and with our program"
- "Importance of R&D in downsizing and in prototyping is obvious and seems to point to a need for more mid-long term, high-risk technology investment"
- ARPA/Marines in the Desert

ARPA and Marines in the Desert

"(We) now have a new set of priorities. Before,...talked about architecture, bits, multichip modules, throughput, etc. Now... are talking about ruggedness, reliability, repairability, friendly interfaces, and a variety of operational uses. It would be difficult to overstate how important these little visits are to us and in the longer term - to the Marines." ***--Dick Urban, May 1993***

“ESTO (GABRIEL & URBAN)
IN THE DESERT WITH THE MARINES”

808-7-2-89-3

30 July 1993

War Games - Completed
(Since 1992 Summer Conference)

- NAVY - NAVWARCOL - Newport, RI
  - 27-29 Jul 92, "Global War Game-92"
  - 3 days - 1 DARPA
- AIR FORCE - AFWARCOL - Maxwell AFB, AL
  - 30 Nov-3 Dec 92, "Global Reach"
  - 5 days - DSRC (Gilbert, Whitesides)
    - DARPA (Alexander, Barker, Buchanan)
- NAVY - NAVWARCOL - Newport, RI
  - 16-20 Nov 92, "SEACON"
  - 5 days - 1 DARPA, 1 ONR

30 July 1993

Exercises & Field Trips - Completed
(Since 1992 Summer Conference)

- AIRFORCE - Tinker AFB, Oklahoma City, OK
  - Oct 92, Jan 93, (Aircraft Maint., Rework, Depot)
  - 2 days
    - DARPA (Coblenz)

- NAVY - NAS Norfolk and NAS Oceana
  - Dec 92, Mar 93, NADEP/AIMD (AirMaint., Rework, Depot)
  - 2 days
    - DSRC (Economy, Heuer, Rapp, Srolovitz)
    - DARPA (Wilcox, Coblenz)
    - ONR (Pohanka, Fishman, Schmidt)

- MARINE CORPS - MCAS Cherry Point
  - Dec 92, Jan 93, (Aircraft Maint., Rework, Depot)
  - 2 days
    - DARPA (Coblenz)

- JOINT/AIR FORCE - Colorado Springs, CO
  - Jan, Jun 93, U.S.Space Command/NORAD/AFSCN
  - 2 days
    - ARPA (Roosild, Alexander, Patterson)
    - DSRC (McGill, Srolovitz)

<u>Exercises & Field Trips - Completed</u>
(Since 1992 Summer Conference)

- MARINE CORPS - 29 Palms, CA
  - Nov 92, May 93 Combined Arms Exercise (CAX) in Desert
  - 3 days - <u>ARPA (Gabriel, Urban, Loda)</u>
- NAVY - Naval Air Station - Whidby Is, WA
  - Sep 92, May 93 EW/EA6B, Attack/A6 Simulator/Rework
  - 2 days - <u>DSRC (C. Evans, McGill, Osgood)</u>
    - <u>ARPA (Durvasula)</u>
    - <u>ONR (Schmidt)</u>
- COALITION/JOINT/MARINE CORPS - Kuwait
  - Jun 93 "Native Fury 93" Exercise in Persian Gulf
  - 7 days - <u>DSRC (Economy)</u>
- NAVY - Naval Air Station - Fallon, NV
  - Jun 93 Carrier Air Wing-Wargame/Exercise prior to BG deploy
  - 2 days - <u>ARPA (Crowley)</u>
    - <u>ONR (Schmidt)</u>

BANGLADESHI ARMY
CLEARING MINE FIELDS
IN KUWAIT

PROFESSOR ECONOMY
AND CAPTAIN LYTIKAINEN
TRYING-OUT THE TECHNIQUE

808-7-2-93-1

**"PROFESSOR OSGOOD AND DR. SCHMIDT-
NAS WHIDBEY ISLAND ,WA"**

808-7-2-93-2

30 July 1993

Exercises & Field Trips

(At 1993 Summer Conference)

A series of 2-4 hr visits to a variety of facilities in the San Diego area were conducted during the Summer Conference. Most were "UNCLAS" visits to enable members awaiting clearance, spouses and dependents to participate.

- NAVY - NAS North Island
  - Naval AirRework Facility (NADEP)
  - 2 trips (1/2 day each) — 7 DSRC
- NAVY - NAS North Island (DSRV/DSV/UMV)
  - Navy Deep Submergence Unit
  - 3 trips (2 hr each) — 8 DSRC, 3 ARPA
- NAVY - NAVSUBBASE Point Loma (attack submarines in port)
  - USS Chicago (SSN-721), USS Topeka (SSN-754)
  - 2 trips (2 hr each) — 12 DSRC, 9 ARPA
- NAVY - NAS North Island (aircraft carriers in port)
  - USS Ranger (CV-61), USS Kitty Hawk (CV-63)
  - 2 trips (2 hr each) — 8 DSRC, 6 ARPA
- NAVAL - NAVPHIBBASE Coronado Island
  - Non-combatant Extraction Ops (NEO) (Sri Lankan/Indian scenario)
  - 1 wargame (1/2 day) — 1 DSRC

July 1993

30 July 1993

DSRC SUMMER CONFERENCE WARGAMING ACTIVITIES

Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
			1	2	3
5	6	7 Deep Submergence Unit North Island	8	9 Naval Air Rework Depot (NADEP) North Island	10 USS Ranger (CV-61) Decommissioning North Island
12	13 USS Chicago (SSN-721) Point Loma	14 USS Kitty Hawk (CV-63) North Island	15 ARPA DAY	16 Deep Submergence Unit North Island	17
19 USS Topeka (SSN-754) Point Loma	20	21 Deep Submergence Unit North Island	22 *GRUNION HUNT*	23 Naval Air Rework Depot (NADEP) North Island Amphibious Wargame Coronado Island	24
26	27	28	29	30 WRAP UP	31

30 July 1993

War Games - Planned

- NAVY - NAVWARCOL - Newport, RI
  - Nov 93 "SEACON/Sea Control"
  - 5 days (science advisor) - 3 ARPA/DSR
    - < Operational/Technology
- AIR FORCE - AFWARCOL - Maxwell AFB, AL
  - 15-19 Nov 93, "Global Reach"
  - 5 days (science advisor) - 8 ARPA/DSRC
    - < Strategic/Regional/Air Power/Technology

30 July 1993

Exercises & Field Trips - Planned

- AIR FORCE - Various ("Blue Two")
  - Aug, Dec 93, Mar, May 94 HazMat, Cold Wx Maint, Fighter/Attack
  - 5 days each — 2 - 3 ARPA/DSRC ea
- MARINE CORPS - 29 Palms, CA
  - Sep 93, Mar, Jun 94, Combined Arms Exercise (CAX) (in desert)
  - 3 days each — 3 - 4 ARPA/DSRC ea
- ARMY - National Training Center - Ft Irwin, CA (in desert)
  - Sep, Nov 93, "OPFOR"/armor/artillery/air/infantry
  - 2 days — 2 - 4 ARPA/DSRC
- MARINE CORPS - Kuwait
  - Jan 94 Coalition/Joint
  - 6 days — 2 - 3 ARPA/DSRC
- ARMY - XVIII Airborne Corps - Ft. Bragg, NC
  - Mar 94, airborne, special operations force exercise
  - 3 days — 2 - 3 ARPA/DSRC
- NAVY - Norfolk, San Diego ("Scientist to Sea")
  - Sep 93-Jun 94 at-sea aboard variety of ships
  - 3-4 days each — 1 - 3 ARPA/DSRC ea

THE SHAPE OF HOLLOW DISLOCATION CORES

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ABSTRACT

Dislocations with large Burgers vectors and elastic constants in crystals with low surface energies have hollow dislocation cores. We analyze the shape of the hollow core and find that it is influenced by anisotropy in both surface energy and elastic constants. Faceted shapes tend to be rotated relative to Gibbs-Wulff shapes. Analogous results should apply for internal precipitates on dislocations.

I. INTRODUCTION

Dislocations with hollow cores have been observed for many years [Verma, 1953]. Often these are the screw dislocations associated with dislocation crystal growth mechanisms. Frank [1951] predicted the size of the hollow core in the case of isotropic elasticity and isotropic (orientation independent) surface energy γ. The change in energy per unit dislocation length associated with forming a hollow core in an isotropic continuous medium is

$$\Delta E = 2\pi R\gamma - \left(\frac{\mu b^2}{4\pi}\right)\ln\frac{R}{r_0} \tag{1}$$

where R is the hollow core radius, μ is the shear modulus, b is the length of the Burgers vector and r_0 is the nonlinear elastic core radius. Here, the matter removed when the hollow dislocation core is formed can be considered to be added to a region remote from the dislocation so that the bulk free energy change per unit volume ΔG_v is zero. The equilibrium hollow core size R^* is set by $(\partial\Delta E/\partial R) = 0$

$$R^* = \frac{\mu b^2}{8\pi^2\gamma} \tag{2}$$

Hence, the hollow core is favored by large μ or b, or by small γ.

The shapes of the hollow cores, for example in the new high T_c oxide superconductors, often deviate from a right circular cylinder and can contain facets. These observations suggest a role of crystal anisotropy in determining the shape. We analyze this possibility, including anisotropic elasticity and orientation-dependent surface energy.

II. WULFF SHAPE

For comparison with the shapes predicted later, we first consider the formation of a void under a uniform driving force. The coordinates system employed in the analysis of a cylindrical

void are shown in Fig. 1. The free energy charge associated with forming a cylindrical void from the continuous medium is

$$\begin{aligned} \Delta E &= \int_0^{2\pi} \gamma(\theta)R(\theta)d\theta - \int_0^{2\pi}\int_0^{R} \Delta G_v r dr d\theta \\ &= \int_0^{2\pi}\left[\gamma(\theta)R(\theta) - \frac{R^2(\theta)}{2}\Delta G_v\right]d\theta \\ &= \int_0^{2\pi} F(\theta)d\theta \end{aligned} \tag{3}$$

Here ΔG_v is the uniform free energy charge per unit volume favoring the formation of the void. ΔG_v can be considered to arise from a uniform strain energy density or from a uniform supersaturation of vacancies.

The equilibrium void shape is found by minimizing the energy ΔE with respect to the void shape $R(\theta)$. This is easily accomplished by setting the functional derivative $\delta\Delta E/\delta R$ to zero and using the Euler equation

$$\frac{\delta \Delta E}{\delta R(\theta)} = 0 = \frac{\partial F}{\partial R(\theta)} = \gamma(\theta) - R(\theta)\Delta G_v \tag{4}$$

which is solved by

$$R(\theta) = \gamma(\theta) / \Delta G_v \tag{5}$$

Hence, in this case, $R(\theta)$, the equilibrium cylindrical void shape, has the same shape as the polar plot of $\gamma(\theta)$, as indicated in Fig. 2. Thus, the use of the Euler equation for the case shown in Fig. 2a reproduces the Gibbs-Wulff plot. When there are cusps in the γ versus θ plot or regions for which $\partial^2\gamma/\partial\theta^2 > 0$, as for the example in Fig. 2c and d, one must use the standard geometrical Wulff construction to determine the equilibrium shape, $R^*(\theta)$.

III. SCREW DISLOCATION - ANISOTROPIC SURFACE ENERGY

We now consider the case of a right-handed screw dislocation coaxial with the void in Fig. 1 so that both **b** and the sense vector ξ points in the + z direction. The free energy change upon forming a core void is

$$\Delta E = \int_0^{2\pi} \gamma(\theta)R(\theta)d\theta - \int_0^{2\pi}\int_{r_0}^{R(\theta)} wr\, drd\theta$$

$$= \int_0^{2\pi} \gamma(\theta)R(\theta)d\theta - \int_0^{2\pi}\int_{r_0}^{R(\theta)} \frac{\mu b^2}{8\pi^2 r^2}\, r\, drd\theta \tag{6}$$

$$= \int_0^{2\pi} F(\theta)d\theta$$

where w is the strain energy density for the screw dislocation and r_0 is the nonlinear elastic core cutoff parameter [Hirth and Lothe. 1982a]. As in the dislocation free case. Eqs. (4)-(5), the equilibrium core void shape is found by minimizing ΔE with respect to $R(\theta)$

$$\frac{\delta \Delta E}{\delta R(\theta)} = 0 = \frac{\partial F}{\partial R(\theta)} = \gamma(\theta) - \frac{\mu b^2}{8\pi^2 R(\theta)} \tag{7}$$

or

$$R(\theta) = \frac{\mu b^2}{8\pi^2 \gamma(\theta)} \tag{8}$$

Performing the second variation of ΔE with respect to $R(\theta)$ indicates that Eq. (5) corresponds to a minimum in ΔE. As for Eq. (2), one could also determine Eq. (8) by setting the sum of the contributions to the chemical potential of a surface atom arising from surface energy and strain energy contributions to zero. The equilibrium dislocation core void shape is of the same form as the <u>dual</u> of the γ plot (i.e.. $R(\theta) \propto 1/\gamma(\theta)$). Figure 3 shows the equilibrium screw dislocation core shape for the anisotropic surface energy $\gamma(\theta)$ of Fig. 2a. Note that the equilibrium dislocation core void shape is rotated by 90° from the void shape in the absence of a screw dislocation (Fig. 2b).

Moreover, as can be readily proven by determining the variations of total energy with θ, the equilibrium shape $R^*(\theta)$ is given by the inner locus of tangents to the $R(\theta)$ plot. Alternatively, one can regard $R(\theta)$ as an effective surface energy and arrive at the same conclusion. As demonstrated in Fig. 4, the consequence is that facets for the screw dislocation case appear at different orientations than for the Gibbs-Wulff shape.

The form of w used in Eq. (6) is strictly valid only for a right circular cylinder shape. As the shape deviates from a right circular cylinder, weak image stresses are needed to satisfy the free surface boundary conditions. However, these are of order r_0^2/R^4 and contain the sine of the angle between the surface normal and R at the point in question. Hence, the correction associated with this effect is small. Since its inclusion would make the problem very complex, we neglect this correction here.

IV. EDGE DISLOCATION - ANISOTROPIC SURFACE ENERGY

For the edge dislocation of Fig. 5, the strain energy density is [Hirth and Lothe, 1982b]

$$w = \frac{\mu b^2}{8\pi^2(1-\upsilon)^2}\left(1-2\upsilon\sin^2\theta\right)\frac{1}{r^2}-\left(\frac{2r_0^2}{r^4}\right) \tag{9}$$

where υ is Poisson's ratio. Here, an image correction (the last term on the right hand side) associated with the free surface boundary condition at R is included, but the weaker effect associated with deviation from a circular cross-section is neglected, as in the previous case. Proceeding as in the screw dislocation case, we find that the equilibrium shape is given by

$$R(\theta) = \frac{\mu b^2(1-2\upsilon\sin^2\theta)}{8\pi^2(1-\upsilon)^2\gamma(\theta)} \tag{10}$$

As for the previous case, $R(\theta)$ is inversely proportional to $\gamma(\theta)$, but it contains added θ dependence in the numerator. The inner locus of tangents construction is valid for this case and, as for Fig. 4, the equilibrium shape $R^*(\theta)$ is rotated relative to the Gibbs-Wulff shape. In this case,

we see that the core image term in Eq. (9) has no effect on the equilibrium shape, providing further justification for the assumption discussed for the screw dislocation case.

V. ANISOTROPIC ELASTICITY

As shown by Foreman [1955], the dislocation field for a screw dislocation has a simple analytical solution if the z axis in Fig. 1 is a 2, 4 or 6 fold axis or conversion axis. This includes the screw dislocation line directions listed in Table I. The explicit elastic solution for this case is given by Hirth and Lothe [1982c]. The strain energy density in this case is

$$w = \frac{b^2}{8\pi^2} \frac{C_{44}C_{55} - C_{45}^2}{C_{44}x^2 - 2C_{45}xy + C_{55}y^2} \tag{11}$$

Here the elastic constants C_{ij} are those rotated into the coordinates x, y, z of Fig. 1. As in the isotropic elastic case, we neglect terms of order r^{-n} with $n \geq 4$ associated with shape deviations from a circle and with the weak elastic constant difference (C_{55}-C_{44}). Analogous to the case of the isotropic edge dislocation, terms of order r^{-4} do not affect the equilibrium shape, so only effects from order n = 6 or higher are ignored for the equilibrium shape: an excellent approximation. Proceeding as before, we find

$$R(\theta) = \frac{b^2}{8\pi^2\gamma(\theta)} \left(\frac{C_{44}C_{55} - C_{45}^2}{C_{44}\cos^2\theta - 2C_{45}\sin\theta\cos\theta + C_{55}\sin^2\theta} \right) \tag{12}$$

Once again, the inner locus of tangents construction applies for the equilibrium shape, $R^*(\theta)$. If C_{44} and C_{55} are substantially different, this could lead to a partially faceted screw dislocation core void. The main effect of varying C_{45} is to rotate the void along the dislocation line direction.

VI. DISCUSSION

The results clearly show that hollow cores with faceted or non-circular cross-sections can be associated with variation in the elastic field with orientation. Moreover, with variations of surface energy with orientation, the equilibrium shape can develop such shape variations even when the

elastic field is invariant with θ. Interestingly, the $R(\theta)$ plot, from which the equilibrium shape is found using the Wulff construction, in the presence of a screw dislocation is the dual of the equilibrium shape of a cylindrical void with no dislocation character.

The latter result can be rationalized as follows. In the absence of surface energy anisotropy, the equilibrium screw dislocation core void is a cylinder of radius inversely proportional to the surface energy (see Eq. 2). This suggests that when the surface energy is low, the core void will have a large radius and vice versa. Therefore, when the surface energy is anisotropic, the low surface energy orientations have an associated large R and the large surface energy orientations have an associated small R. This creates a core void in which more of the surface has high surface energy orientations than low surface energy orientations. This is exactly opposite to what happens in the absence of a dislocation, where the equilibrium void surface tends to have a relatively greater abundance of low energy orientations than high energy orientations. This is the reason for the rotation of the equilibrium void shape with and without the dislocation for a fixed $\gamma(\theta)$ (cf. Figs. 2b and 3).

Acknowledgments: The authors are grateful for the support of this research in part by the Advanced Research Project Agency through the Office of Naval Research Contract N00014-92-C-0143 with Charles Evans and Associates, Redwood City, Ca.

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TABLE I

Examples of Screw Dislocations Axes for Which Eq. (11) Applies

Crystal System	Axis Direction
Cubic	<001>, <011>
Tetragonal, general	[001]
4/m, 4mm	[100], [010]
422	[110]
Hexagonal	[0001], $\langle 10\bar{1}0]$, $\langle 11\bar{2}0]$
Rhombohedral 32 or 3m	$\langle 10\bar{1}0]$
Orthorhombic	<001>
Monoclinic	[001]

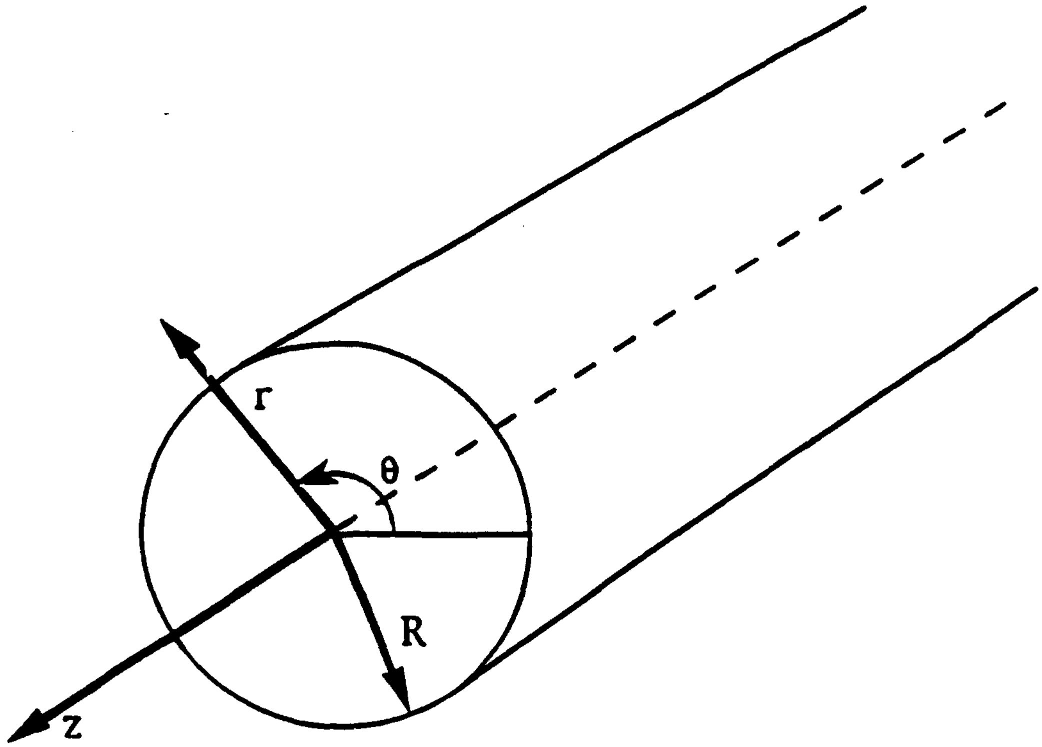
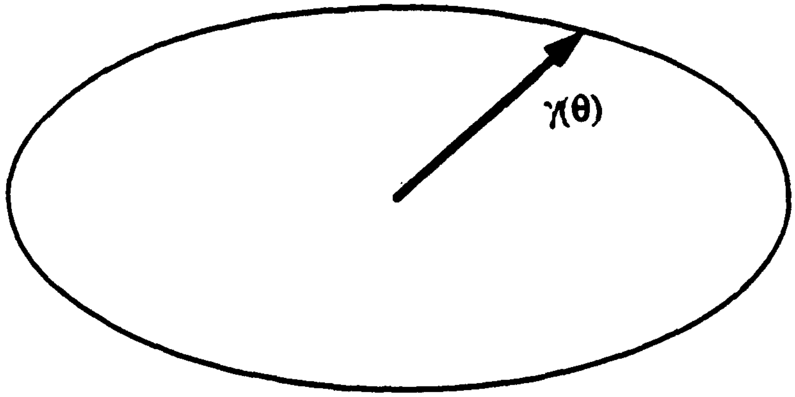
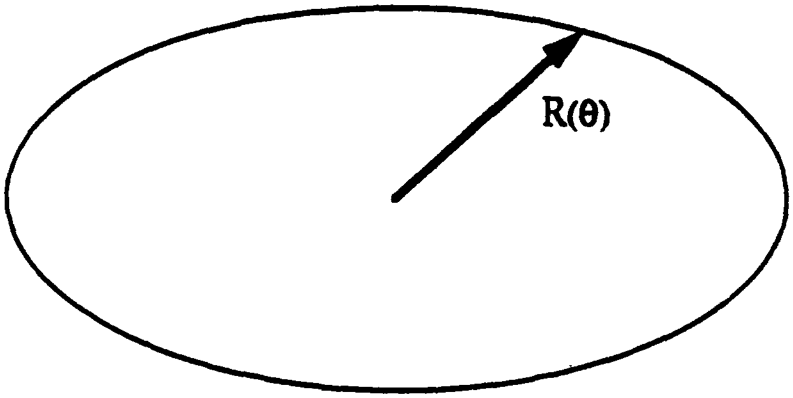


Figure 1 Cylinder with axis parallel to z axis.

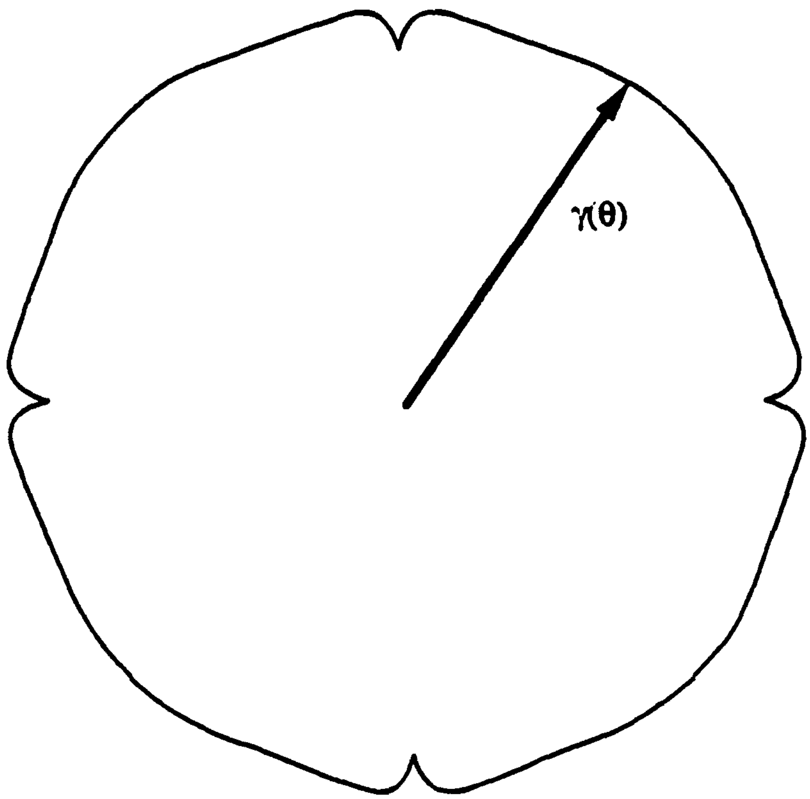
2a



2b



2c



2d

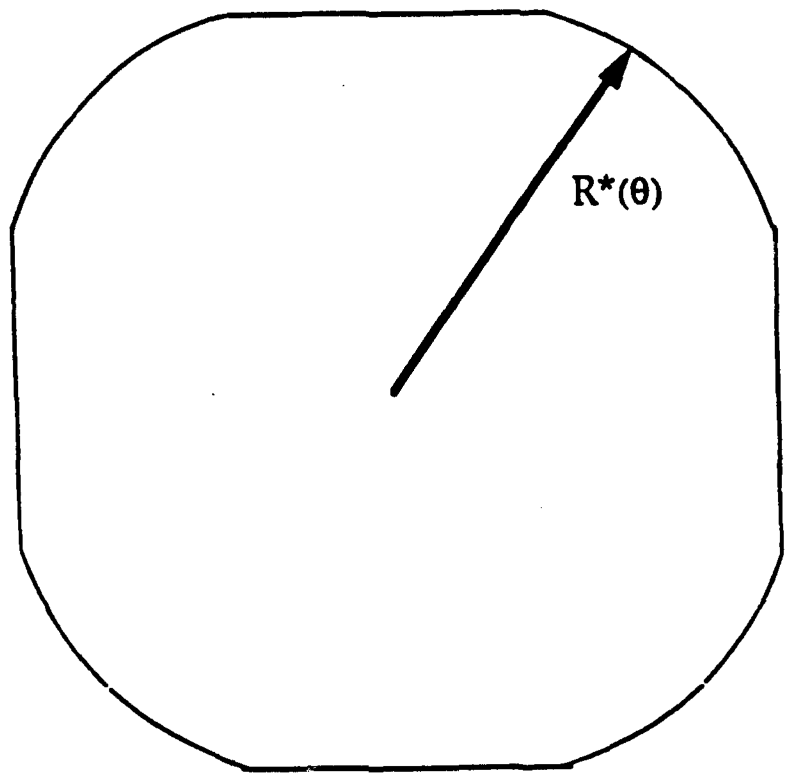


Figure 2 Polar plots of two different $\gamma(\theta)$ functions (a and b) and the corresponding equilibrium shapes (c and d).

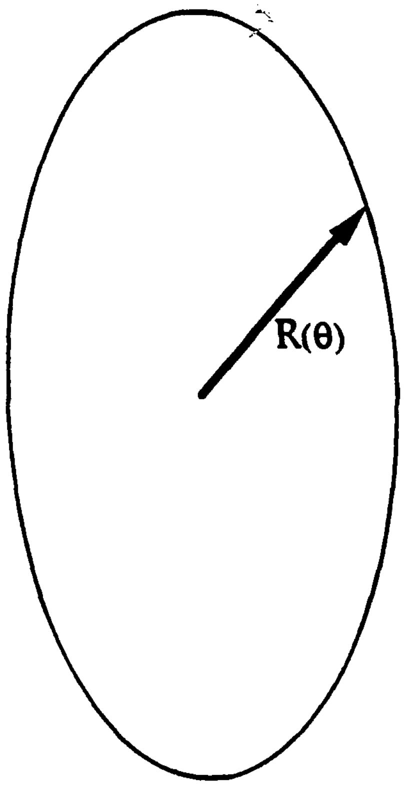
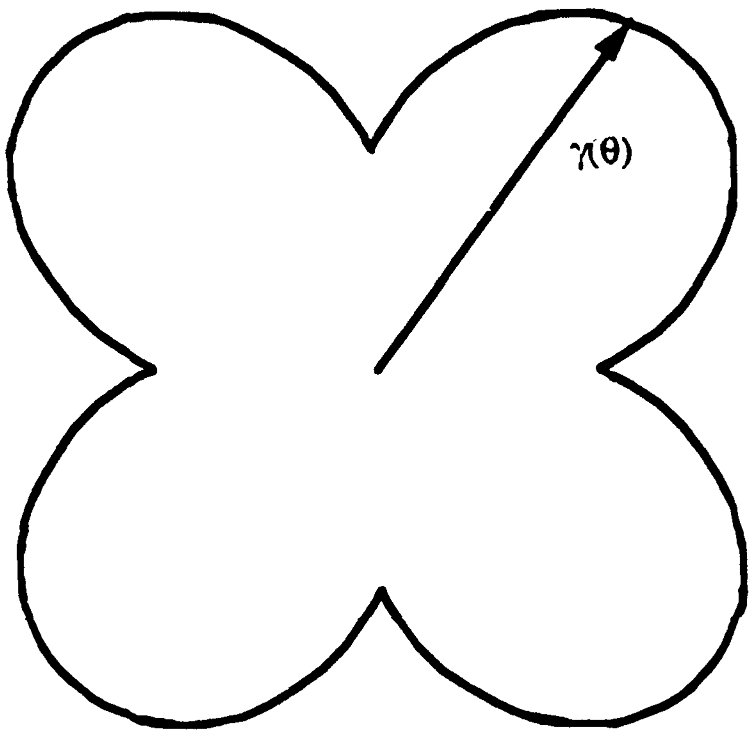
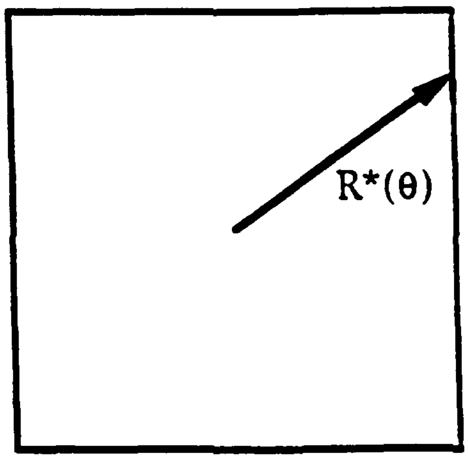


Figure 3 Polar plot of equilibrium screw dislocation core shape $R^*(\theta)=R(\theta)$ for the $\gamma(\theta)$ function of Fig. 2a.

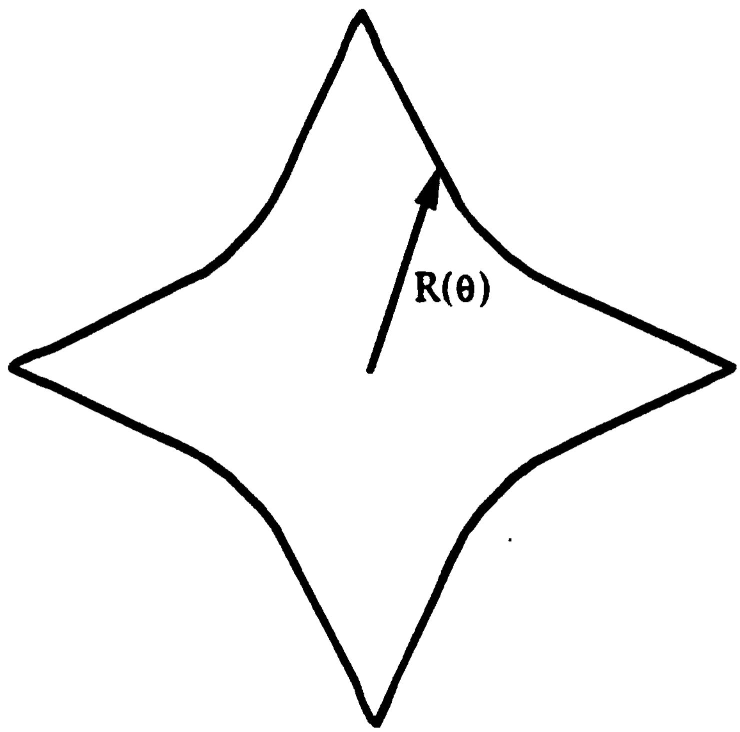
4a



4b



4c



4d

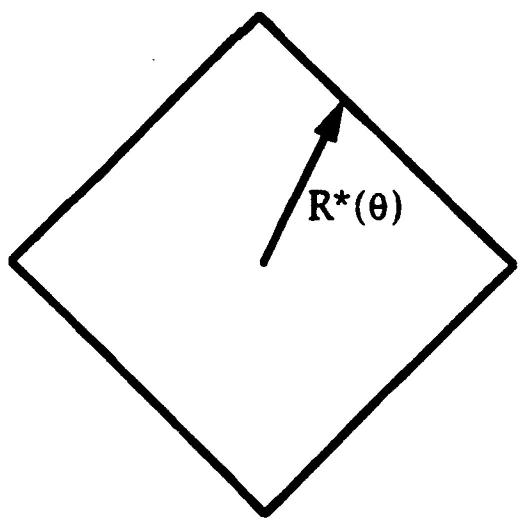


Figure 4 Plot of (a) $\gamma(\theta)$ and (b) the corresponding equilibrium void shape in the absence of a dislocation. Plot of (c) $R(\theta)$ for the $\gamma(\theta)$ in (a) and (d) the corresponding equilibrium core void shape in the presence of a screw dislocation.

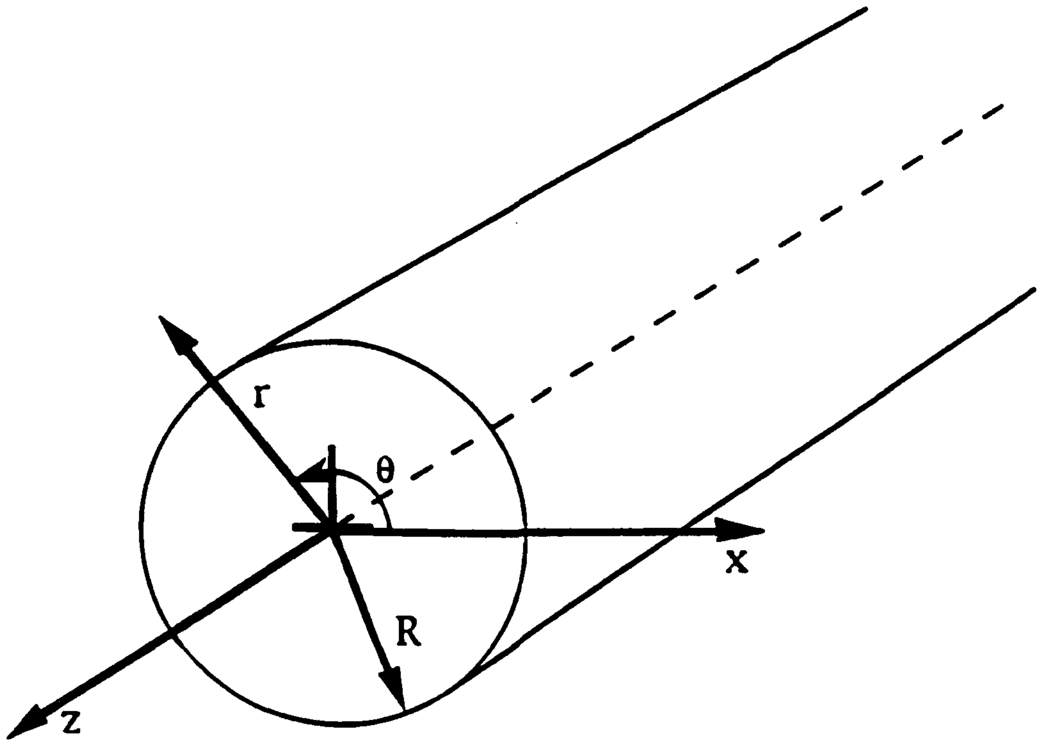


Figure 5 Edge dislocation with a cylindrical void at its core.

INTRINSIC STRESSES IN CVD FILMS

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and D. R. Clarke

EXECUTIVE SUMMARY

Background

When a vapor-deposited polycrystalline film is grown on a substrate having an incoherent interface, there is no obvious mechanism for generating stress in the surface layer as it deposits. Surface diffusion allows atom displacements which relax strains as they attempt to develop. This situation differs from that for coherent, single crystal films which incur coherency strains.

Intrinsic stresses usually develop as a consequence of subsequent diffusional effects that occur in previously deposited sections of the film. This involves mechanisms which eliminate those defects present in the film which have an associated 'free volume.' The one exception is the stress associated with surfaces and interfaces, discussed below.

The films of interest have a thin, equiaxied polycrystalline nature close to the interface. Above this layer, a columnar grain structure develops with a preferred crystallographic orientation. A common experience is that the equiaxied layer has a higher residual stress than the columnar material, resulting in bending when the film is removed from the substrate. Typical bending strains are of order 2×10^{-4}, indicating a stress differential between these regions of order 80 MPa.

Intrinsic stresses in films are generally in the range 0.5 to 4 GPa. They can be tensile or compressive. They are also superposed on thermal expansion mismatch stresses. The mechanisms to be considered emphasize phenomena capable of giving GPa level stresses. Furthermore, the defects that give rise to the stresses, as they are eliminated by diffusion, must have sufficient density to

provide the misfit strain, ε, which governs the intrinsic stress σ_I, through the relation

$$\sigma_I = E\varepsilon/3(1-\nu)$$

Mechanisms

There are numerous potential mechanisms for intrinsic stress development. Emphasis is given to the six mechanisms that may operate in inorganic films produced by CVD.

(i) Grain Growth

The grain boundary is a source of 'free-volume' that diminishes as the grains grow, subsequent to deposition. As a small grain disappears (Fig. 1), stresses are set up. These stresses provide a strain energy contribution to the chemical potential of the atoms on the two sides of a grain boundary. The transformation strain associated with the process depicted in Fig. 1, is

$$\varepsilon = 6\Delta a\left(\frac{1}{d} - \frac{1}{d_o}\right) \tag{1}$$

where d is the actual grain size, d_o is the initial value as the film deposits, Δa is the grain boundary free volume per unit area (which is of order the atomic dimension). The contribution of the strain energy to the chemical potential difference is

$$\Delta\mu_s = \frac{1}{2}E\varepsilon^2\Omega \tag{2}$$

where Ω is the atomic volume and E is Young's modulus. This potential adds to that from the grain boundary curvature

$$\Delta\mu_b = (2\gamma_b/d)\Omega \tag{3}$$

By setting the potential difference to zero, there is an equilibrium residual stress, σ_{eq} which occurs at an equilibrium grain size, d_{eq}. Of course, the temperature needs to be large enough to allow grain boundary diffusion at a sufficiently rapid rate to attain this equilibrium. The equilibrium values are

$$\sigma_{eq} = 3\gamma_b/2(\Delta a) \tag{4a}$$

and

$$\Delta d_{eq} = \frac{3(1-\nu)d^2\gamma_b}{4E(\Delta a)^2} \tag{4b}$$

Typical values are:

$$\sigma_{eq} \approx 1 - 4\text{GPa},\ d_{eq} \approx 5 - 20\ \mu\text{m}.$$

Note that these stresses develop with time at temperature, by grain boundary diffusion, and they *cannot* be eliminated by heat treatment. Moreover, higher stresses are more likely in fine grained material, which has a higher initial motivation for grain growth. Only tensile stress can develop.

For this mechanism to apply to CVD films, it would be necessary for the grains that form during deposition to be quite small and then grow into the classical configurations found when deposition is complete. Previously, this has been considered unlikely, because the evolution from equiaxied to columnar has been regarded as a natural growth mode for deposited film. Nevertheless, this possibility can be tested using methods discussed below.

The misfit strain required to achieve the equilibrium stress (eqn. 4) is of order, $\varepsilon \approx 5 \times 10^{-3}$. Such stress can be achieved by removing at least one lateral grain boundary from each ~0.5μm of film.

(ii) Point Defect Annihilation

If point defects are trapped in the film as it grows, their subsequent elimination at either grain boundaries or dislocations can cause intrinsic stress. The annihilation of vacancies or interstitials at grain boundaries is entirely analogous to dislocation climb (Fig. 2). The chemical potentials in the system are:

$$\Delta\mu = \sigma_n\Omega + kT\ell nC/C_o \tag{5}$$

where C/C_o is the excess point defect concentration, and σ_n is the stress normal to the boundary. There is an equilibrium intrinsic stress at $\Delta\mu = O$, given by

$$\sigma_{eq} = \left(\frac{kT}{\Omega}\right)\ell nC/C_o \tag{6}$$

If $C/C_o \approx 2$, $\sigma_{eq} \approx 2$ GPa.

This stress develops with time at temperature. It requires lattice diffusion and thus occurs *slowly*. Once present, the stresses cannot be eliminated. Instead, they may increase upon annealing. These stresses can be either tensile (vacancies) or compressive (interstitials). There is no obvious grain size effect on the stress. However, the stresses develop more rapidly in small grained films, because the diffusion distances are smaller.

In order to develop equilibrium level intrinsic stresses, misfit strains of $\sim 10^{-3}$ must be possible. This requires an original point defect concentration in the film, as it grows, $C_v \approx 10^{-3}$. This represents a very high supersaturation, which would be detectable by several different experiments.

(iii) Hydrogen Effects

When hydrogen is a product of the CVD reaction, there will be large H activity at the film surface (Fig. 3). This H may either diffuse into the film or may be trapped during growth. The potential at any point in the film is

$$\Delta\mu = kT \ln C_H/C_o - \sigma\Omega_H \qquad (7)$$

where Ω_H is the partial molar volume of H and C_H is the concentration relative to the equilibrium value C_o. A flux of H that causes C_H to deviate from the initial state creates residual stress, which tends to suppress further diffusion. There is an equilibrium stress, at final concentration C_H^* given by,

$$\sigma_{eq} = \frac{kT}{\Omega_H} \ln C_H^*/C_H^o \qquad (8)$$

where C_H^o is the hydrogen concentration in the film, as it deposits. Typical values of σ_{eq} are 1–4 GPa.

The rate of stress development depends on the hydrogen diffusivity D_H, as well as the film thickness. The stress develops more rapidly when the film is thin. The stresses are compressive if H diffuses into the film, but tensile if H is trapped during growth and then diffuses out. For the former, subsequent annealing may reduce the stress, by causing the H to diffuse out.

For equilibrium stresses to be reached, the misfit strain is

$$\varepsilon \approx C_H\Omega_H \approx 10^{-3}$$

Since Ω_H is probably small for diamond, a very high concentration of H is needed to give high stresses.

(iv) Sintering

Voids present on the grain boundaries upon deposition can be eliminated by subsequent sintering to create a residual tensile stress (Fig. 4). This stress has a maximum value

$$\sigma_{eq} = 2\gamma_s/R \tag{9}$$

where γ_s is the surface energy and R is the void radius. Typical values range between 20 MPa for 0.1 µm voids to 2 GPa for 1nm voids. To achieve the required misfit stress, a void volume fraction, $f \approx 10^{-3}$ would be needed on the as-deposited grain boundaries.

v) Grain Boundary Stress

There is a stress associated with the grain boundaries (Fig. 5). This stress is given by

$$\sigma = \gamma_b/d \tag{10}$$

It is typically 1 MPa for 1 µm size grain. Nanometer size grains are needed for this stress to be important.

(vi) Temperature Gradients

If the temperature at the deposition surface changes as the film grows, there will be an associated residual stress. The stress difference through the film is given by

$$\Delta\sigma = E_f \alpha_f \Delta T \tag{11}$$

where α_f is the thermal expansion coefficient for the film and ΔT is the variation in deposition temperature.

Measurements

(i) Residual Stress

Beam bending measurements can give different values of residual stress than lattice strain techniques (x-ray, Raman spectroscopy). For example, the grain boundary stress causes beam bending but no lattice strain. Conversely, lattice stress may exist because of point defects, but there is no beam bending.

The beam bending force is the measure of residual stress *relevant* to CVD diamond films.

(ii) Point Defects

The point defect concentration could be measured by quenching the film at various stages during growth, by using a helium jet. The point defect content may then be obtained by EPR and luminescence measurements. It can also be obtained from dislocation loop shrinkage rates, measured in the TEM.

(iii) Grain Size

The grain size that exists *in situ* during film growth might be monitored by optical scattering measurements made on the film surface. These measurements would be compared with post *situ* TEM measurements to address grain growth during film deposition.

Diamond Films

The literature on CVD diamond films indicates several key features (Fig. 6) (i). The initial ~ 1/2 μm is stress free. (ii) The next several microns are subject to an intrinsic tensile stress. (ii) This stress increases as the deposition temperature increases. (iv) The grain size increases as the deposition temperature increases, from ~1μm at 700C to ~5μm at ~ 900C. (v) After removal from the substrate, the film bends with a sign that suggests reduced residual tension in the columnar region.

A working hypothesis based on these 'facts' is as follows. The columnar region is nominally stress-free. The equiaxied region has an intrinsic stress $\sigma_s \approx 600$ MPa. The bending strain is then

$$\varepsilon_b = 3(w/t)(\sigma_s/E) \tag{12}$$

where w is the thickness of the equiaxied zone and t is the total thickness. If $w \approx 50\ \mu m$ and $t \approx 1$ mm, then $\varepsilon_b \approx 10^{-3}$, consistent with the bending found experimentally.

Since the intrinsic stress increases as the temperature of deposition increases and as the grain size in the equiaxed region increases, the grain growth mechanism appears to be the most plausible. Specifically, the grains in this zone, as deposited, are submicron in size. They grow as the columnar region is deposited to an extent that increases as the temperature increases. The more extensive the grain growth, the higher the residual tension.

If this hypothesis is correct, the preferred solution is to control the nucleation stage on the substrate to prevent the formation of small equiaxied grains as the first layers deposit.

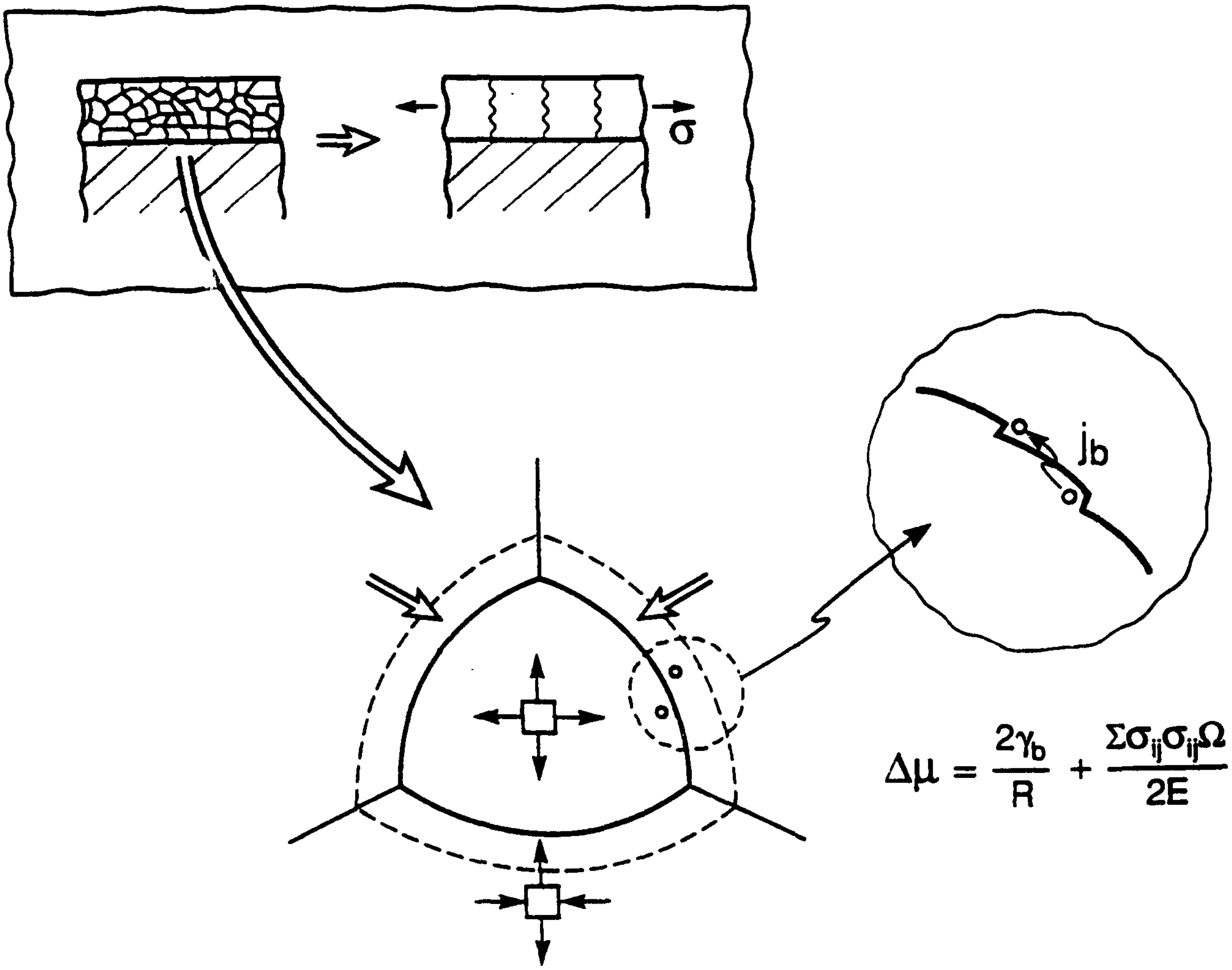


Fig. 1 Grain Growth Mechanism

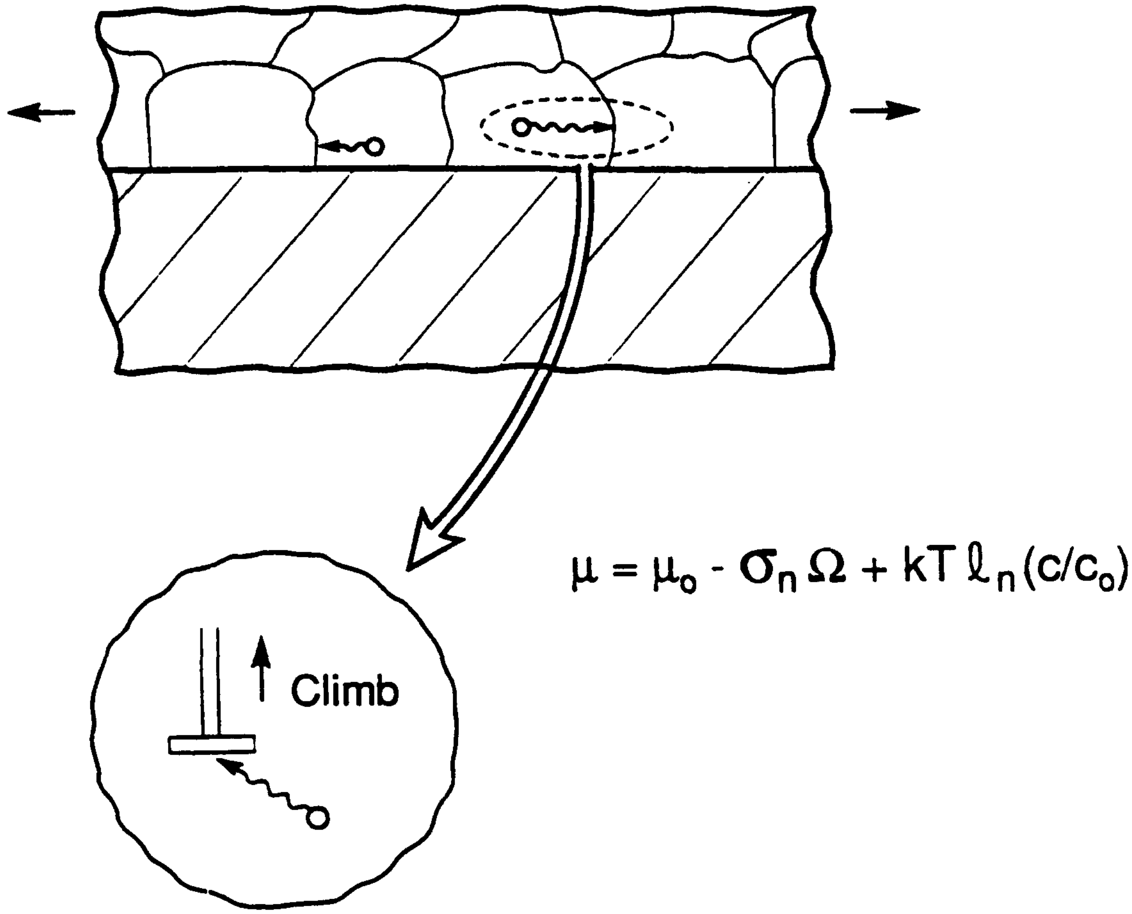


Fig. 2 Point Defect Anihilation Mechanism

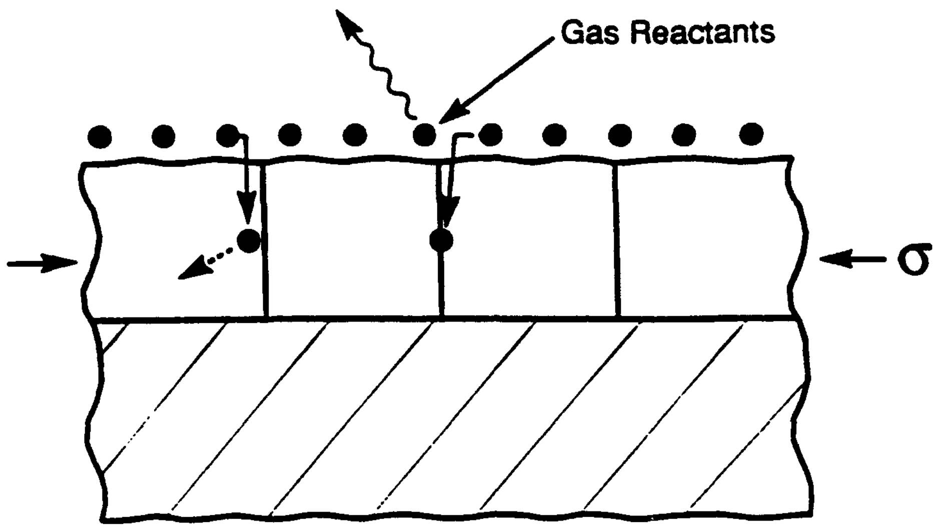


Fig. 3 Hydrogen Ingress Mechanism

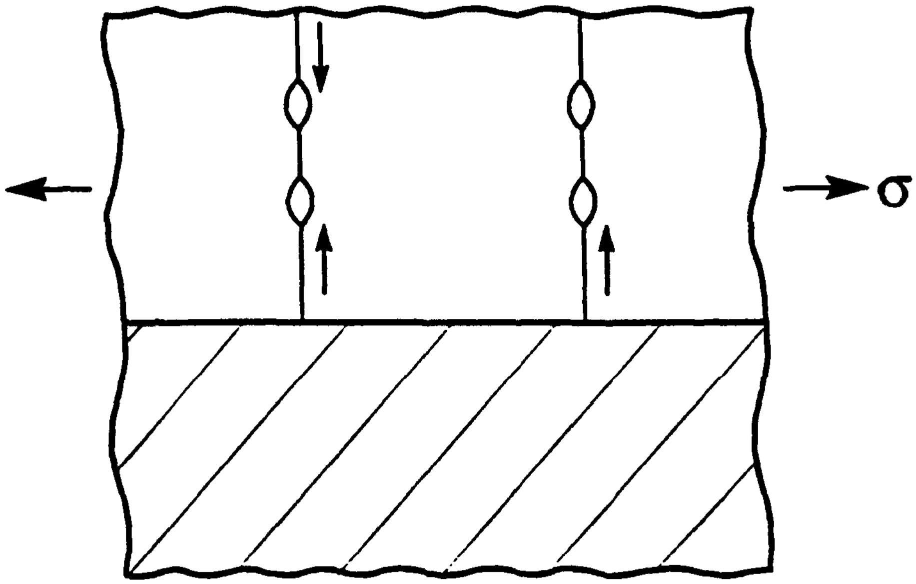


Fig. 4 Sintering

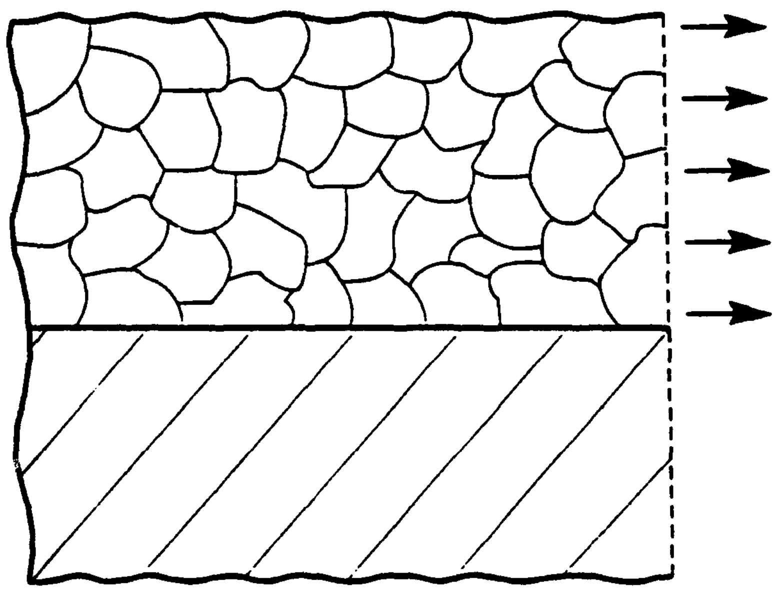
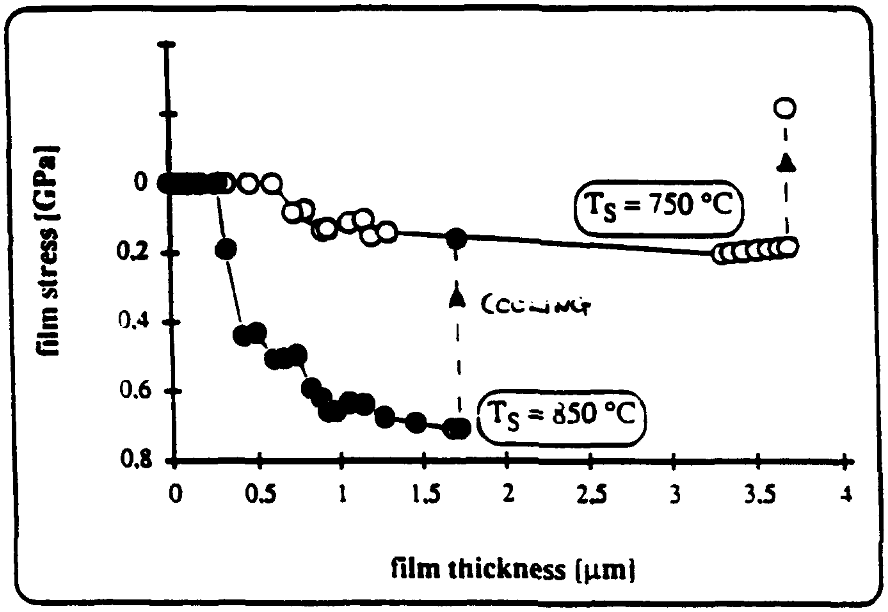
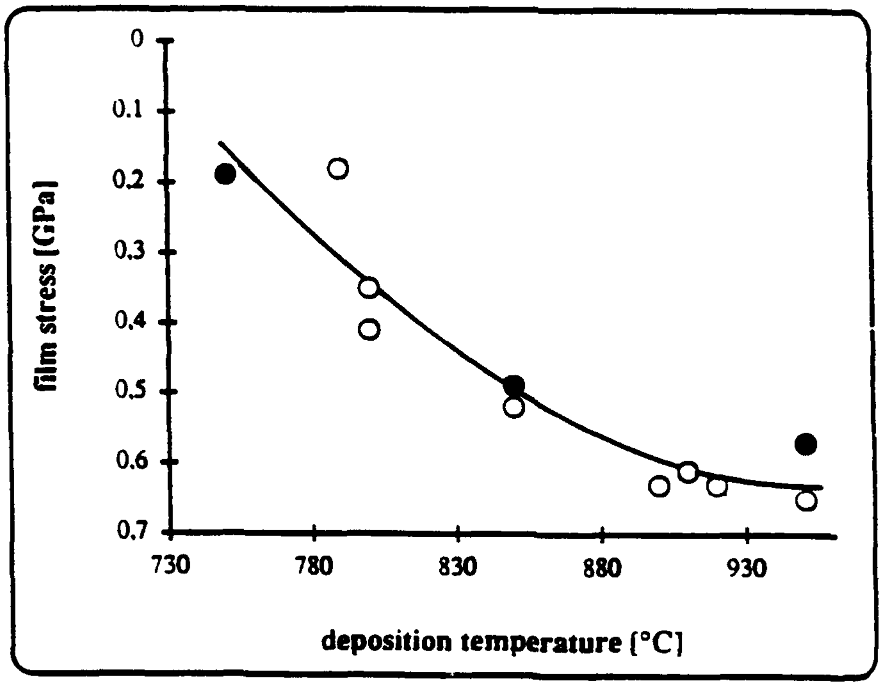


Fig. 5 Grain Boundary Stress



film stress [GPa]
0
0.2
0.4
0.6
0.8
T_S = 750 °C
T_S = 850 °C
0
0.5
1
1.5
2
2.5
3
3.5
4
film thickness [μm]



film stress [GPa]
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
730
780
830
880
930
deposition temperature [°C]